10/730,643

FILE 'HOME' ENTERED AT 09:00:10 ON 28 DEC 2004

=> file reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 09:00:17 ON 28 DEC 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 26 DEC 2004 HIGHEST RN 802853-20-9
DICTIONARY FILE UPDATES: 26 DEC 2004 HIGHEST RN 802853-20-9

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

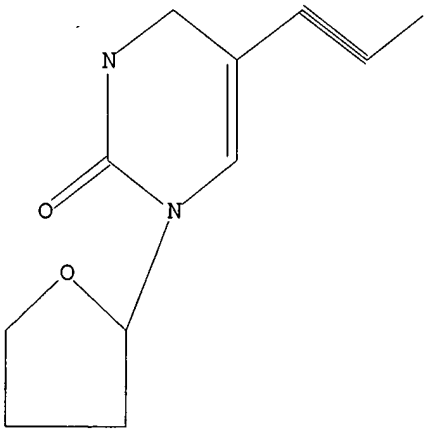
Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

*** YOU HAVE NEW MAIL ***

=>
Uploading C:\Program Files\Stnexp\Queries\10730643.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

```
=> s l1 full
FULL SEARCH INITIATED 09:00:37 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   2211 TO ITERATE

100.0% PROCESSED    2211 ITERATIONS                          1171 ANSWERS
SEARCH TIME: 00.00.01

L2          1171 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               155.42     155.63

FILE 'CAPLUS' ENTERED AT 09:00:43 ON 28 DEC 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)
```



```
FILE COVERS 1907 - 28 Dec 2004  VOL 142 ISS 1
FILE LAST UPDATED: 24 Dec 2004  (20041224/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.
```

=> d l9 bib abs hitstr 1-15

L9 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:31284 CAPLUS
DN 132:78806
TI Oligonucleotide-polyamide conjugates for use as PCR primers and hybridization probes
IN Tregear, Geoffrey William; Haralambidis, Jim
PA Howard Florey Institute of Experimental Physiology and Medicine, Australia
SO U.S., 22 pp., Cont.-in-part of U.S. 5,552,540.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 3

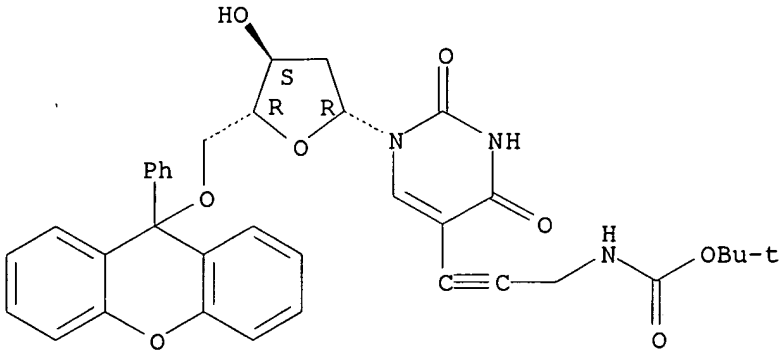
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6013434	A	20000111	US 1995-343535	19950209
	US 5552540	A	19960903	US 1993-68604	19930527
	WO 9324511	A1	19931209	WO 1993-AU252	19930528 <--
	W: AU, JP, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
PRAI	US 1989-457747	B1	19891222		
	AU 1992-2682	A	19920529		
	US 1993-68604	A2	19930527		
	WO 1993-AU252	W	19930528		
	AU 1987-2666	A	19870624		
	US 1993-477995	A2	19930424		

AB This invention relates to novel oligonucleotide-polyamide conjugates preferably having a free 3'-hydroxyl moiety, and wherein the polyamide is coupled to the oligonucleotide through its carboxyl terminus. Nucleotide polymer conjugates Nu-NUC-C.tplbond.C-X1-NH-X2-X3 [X1 is an unsubstituted or substituted C1-C10 alkylene group, in which one or more carbons may optionally be replaced by -NH-, -O- or -S-; X2 is a bond, or an unsubstituted or substituted C1-C20 alkylene group, in which one or more carbons may optionally be replaced by -NH-, -O- or -S-; X3 is an amino acid, or a polyamide linked via its carboxy terminus; NUC is a nucleoside group; Nu is an oligonucleotide] are reported. Methods of preparing these compds., and various uses, for example, as PCR primers, or as a substrate for DNA or RNA polymerase, are also disclosed.

IT **146954-81-6DP**, controlled-pore glass-bound **146954-81-6P**
146954-82-7DP, controlled-pore glass-bound **146954-82-7P**
146954-88-3DP, controlled-pore glass-bound
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(oligonucleotide-polyamide conjugates for use as PCR primers and hybridization probes)

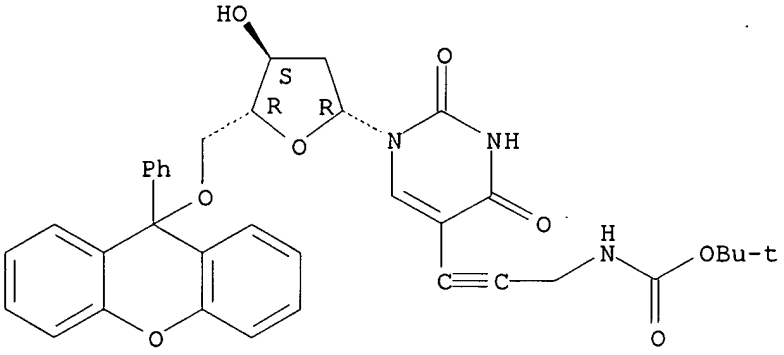
RN 146954-81-6 CAPLUS
CN Carbamic acid, [3-[1-[2-deoxy-5-O-(9-phenyl-9H-xanthen-9-yl)-β-D-erythro-pentofuranosyl]-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]-2-propynyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



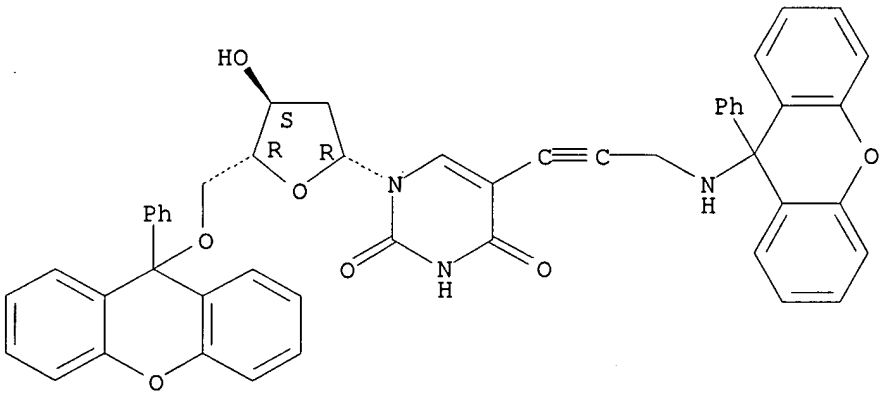
RN 146954-81-6 CAPLUS
CN Carbamic acid, [3-[1-[2-deoxy-5-O-(9-phenyl-9H-xanthen-9-yl)-β-D-erythro-pentofuranosyl]-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]-2-propynyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



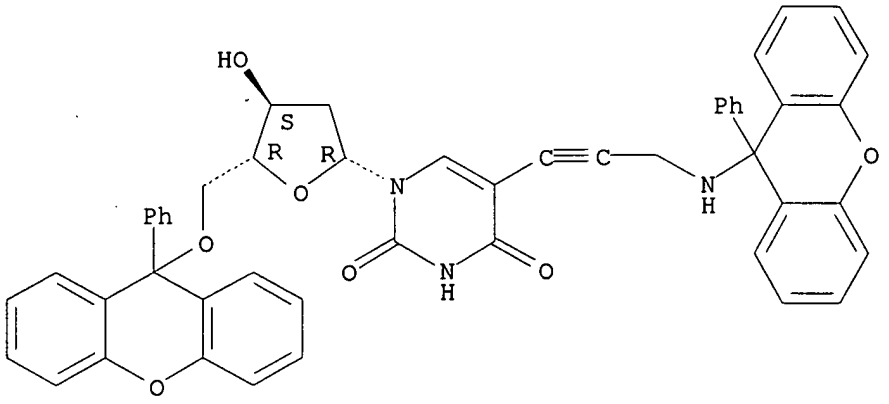
RN 146954-82-7 CAPLUS
CN Uridine, 2'-deoxy-5'-O-(9-phenyl-9H-xanthen-9-yl)-5-[3-[(9-phenyl-9H-xanthen-9-yl)amino]-1-propynyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 146954-82-7 CAPLUS
CN Uridine, 2'-deoxy-5'-O-(9-phenyl-9H-xanthen-9-yl)-5-[3-[(9-phenyl-9H-xanthen-9-yl)amino]-1-propynyl]- (9CI) (CA INDEX NAME)

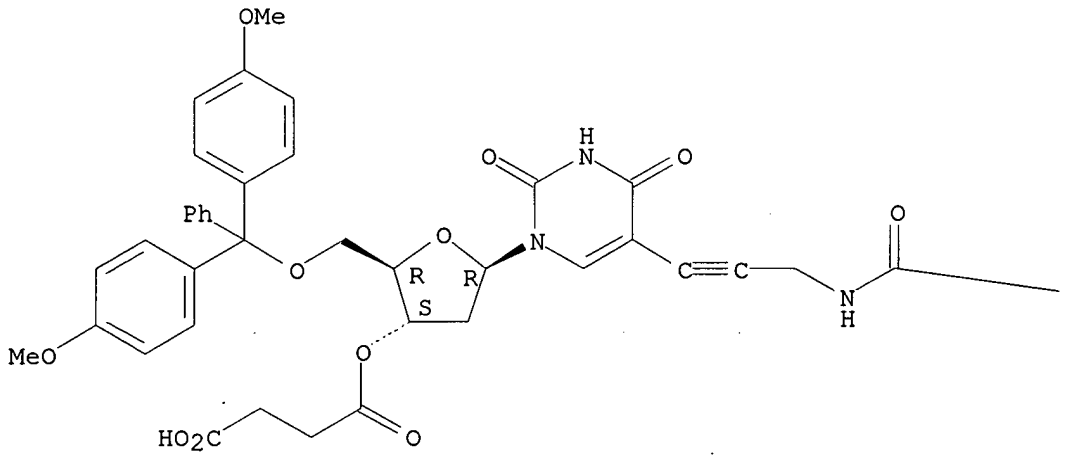
Absolute stereochemistry.

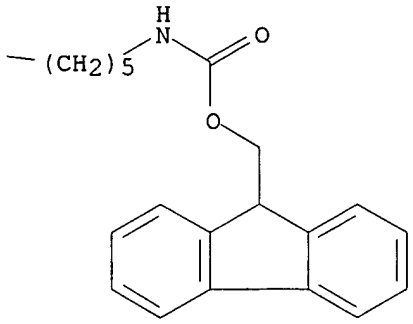


RN 146954-88-3 CAPLUS
CN Carbamic acid, [6-[[3-[1-[5-O-[bis(4-methoxyphenyl)phenylmethyl]-3-O-(3-carboxy-1-oxopropyl)-2-deoxy-β-D-erythro-pentofuranosyl]-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]-2-propynyl]amino]-6-oxohexyl]-, mono(9H-fluoren-9-ylmethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

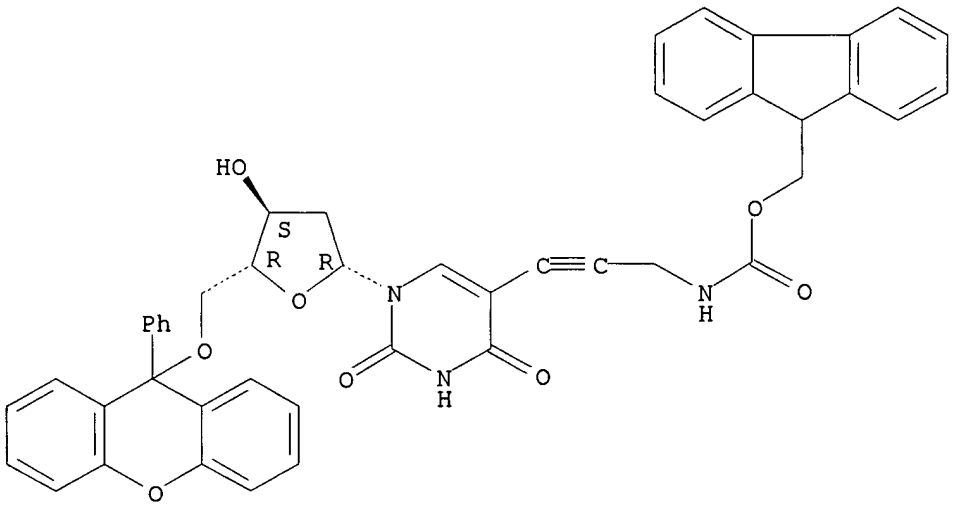
PAGE 1-A





IT **146954-80-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(oligonucleotide-polyamide conjugates for use as PCR primers and hybridization probes)
RN 146954-80-5 CAPLUS
CN Carbamic acid, [3-[1-[2-deoxy-5-O-(9-phenyl-9H-xanthen-9-yl)-β-D-erythro-pentofuranosyl]-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]-2-propynyl]-, 9H-fluoren-9-ylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

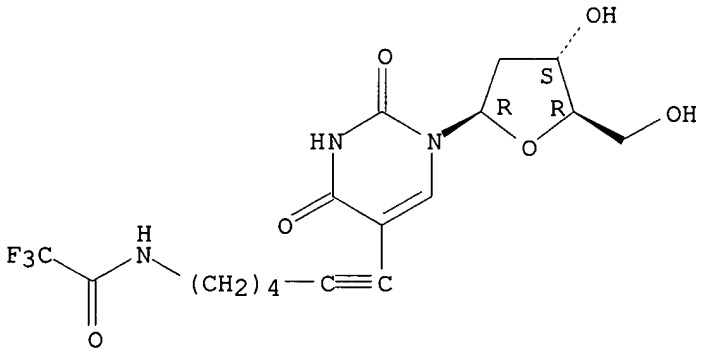


RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1993:650367 CAPLUS
DN 119:250367
TI Zwitterionic DNA
AU Hashimoto, Hiromasa; Nelson, Marek G.; Switzer, Christopher

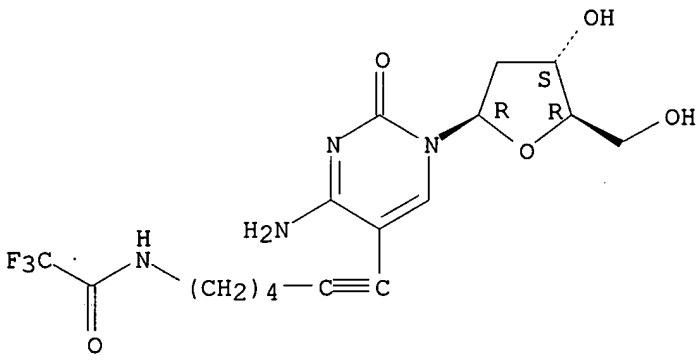
CS Dep. Chem., Univ. California, Riverside, CA, 92521, USA
SO Journal of the American Chemical Society (**1993**), 115(16), 7128-34
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
AB As a strategy to make DNA net charge neutral, oligodeoxyribonucleotides bearing pyrimidine 5-ω-aminohexyl substituents have been synthesized and characterized. The resultant zwitterionic oligomers bind to the natural DNA at low ionic strength as well or better than does natural DNA with itself, even when all of the nucleotides in a given single strand are rendered zwitterionic. As would be expected, stabilities of duplexes bearing zwitterionic strands are relatively insensitive to changes in solution ionic strength as compared with natural DNA. Somewhat surprising, however, is the finding that a DNA duplex composed of a fully zwitterionic strand and a natural complementary strand exhibits no change in stability over a 20-fold change in ionic strength. Thus, double- and single-stranded states in this case have equivalent charge densities, consistent with the zwitterionic strand contributing no net charge. Stabilization due to the ammonium ions was verified by comparing free energies of DNA duplexes bearing hexyl tethered ammonium ions with those bearing simply hexyl groups devoid of ammonium ions. This comparison showed that without an added pos. ammonium ion, the hexyl tether itself has a severe and cumulative unfavorable effect on duplex stability. Finally, zwitterionic nucleotides are found to distinguish matched from mismatched nucleotides in cDNA strands to a degree that rivals natural DNA.
IT **149798-20-9P 149798-21-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenation of)
RN 149798-20-9 CAPLUS
CN Uridine, 2'-deoxy-5-[6-[(trifluoroacetyl)amino]-1-hexynyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 149798-21-0 CAPLUS
CN Cytidine, 2'-deoxy-5-[6-[(trifluoroacetyl)amino]-1-hexynyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

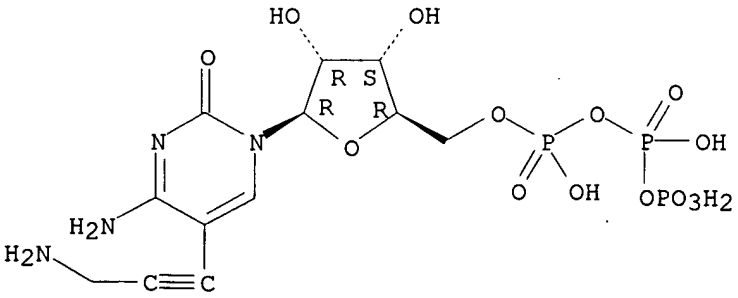


L9 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1993:597261 CAPLUS
DN 119:197261
TI Method for preparing probes for **nucleic acid** identification
IN Takenishi, Soichiro; Suzuki, Osamu; Yokomizo, Hirohiko; Shoji, Tomotoshi; Ooyama, Akihiro; Ishimaru, Mika
PA Nisshin Spinning, Japan
SO Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 05184395	A2	19930727	JP 1992-26217	19920116 <--
PRAI JP 1992-26217		19920116		

OS MARPAT 119:197261
AB The method comprises enzyme polymerization of the functional group-containing derivs. of nucleoside triphosphate, and incorporation of label through functional group binding for preparing probe for DNA determination The nucleoside triphosphate derivs. contain nitro, sulfonyl, amino, hydroxy, mercapto, carboxy, aldehyde, etc. Thus, 5-(3-aminopropyl)cytidine-5'-triphosphate was used for preparing fluorescein-label RNA probe for mouse NFG gene. 5-(3-Aminopropyl)-2'-deoxyuridine-5'-triphosphate was used for preparing DNA probe.
IT **150718-26-6P**
RL: PREP (Preparation)
(preparation of RNA probe with)
RN 150718-26-6 CAPLUS
CN Cytidine 5'-(tetrahydrogen triphosphate), 5-(3-amino-1-propynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L9 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1993:118248 CAPLUS
DN 118:118248
TI **Nucleic acid** sequence analysis with nucleoside-5'-O-(1-thiotriphosphates)
IN Lee, Linda J.
PA Applied Biosystems, Inc., USA
SO PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

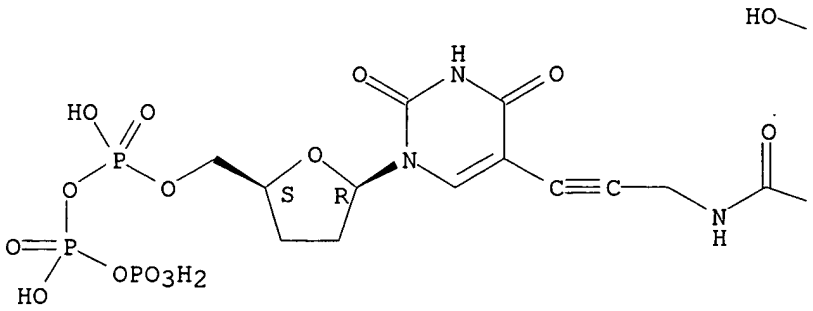
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	WO 9206219	A1	19920416	WO 1991-US7345	19910927	<--
	W: JP					
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE					
	US 5187085	A	19930216	US 1990-590218	19900928	<--
	EP 550646	A1	19930714	EP 1991-918268	19910927	<--
	EP 550646	B1	20000405			
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE					
	JP 05507000	T2	19931014	JP 1991-517034	19910927	<--
	JP 06061280	B4	19940817			
	AT 191511	E	20000415	AT 1991-918268	19910927	
PRAI	US 1990-590218	A	19900928			
	WO 1991-US7345	W	19910927			

AB A chain-terminating method of **nucleic acid** sequencing in which comprises an oligonucleotide primer is extended with a **nucleic acid** polymerase in a reaction mixture containing nucleoside-5'-O-(1-thiotriphosphate) precursors and ≥1 chain-terminating nucleotide is described. The resulting DNA fragment products have more uniform bands as seen after electrophoresis and therefore give more accurate base determination Preparation of chain-terminating dideoxynucleotides labeled with different dyes selected from rhodamines and fluoresceins was shown. Sequence determination using rhodamine-labeled dideoxynucleotides, nucleoside-5'-O-(1-thiotriphosphate) precursors, and Sequenase (a T7 DNA polymerase) in a Mn++-containing buffer was also described.

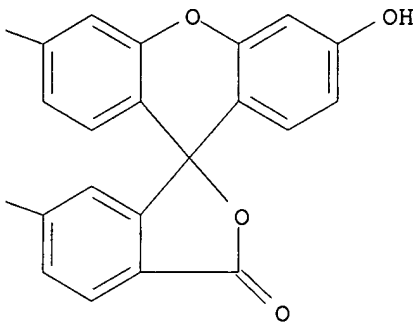
IT **142975-54-0D**, conjugate with dideoxynucleosides
142975-63-1D, conjugate with dideoxynucleosides
RL: USES (Uses)
(in DNA sequencing by chain termination, nucleoside thiotriphosphates for improved band uniformity and accuracy in)
RN 142975-54-0 CAPLUS
CN Uridine 5'-(tetrahydrogen triphosphate), 2',3'-dideoxy-5-[3-[[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-6-yl)carbonyl]amino]-1-propynyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

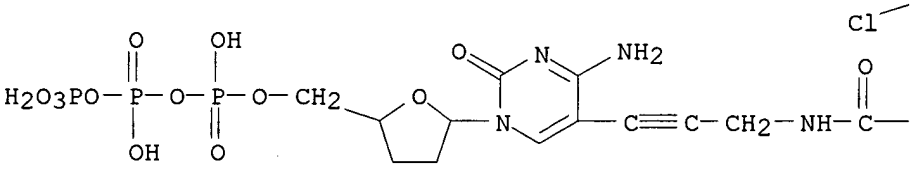


PAGE 1-B

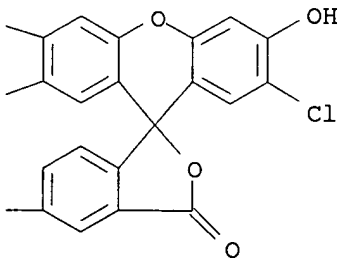


RN 142975-63-1 CAPLUS
CN Cytidine 5'-(tetrahydrogen triphosphate), 2',3'-dideoxy-5-[3-[[(2',7'-dichloro-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)carbonyl]amino]-1-propynyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

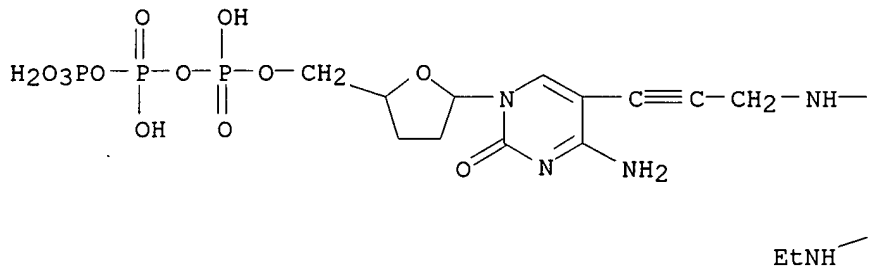


PAGE 1-B

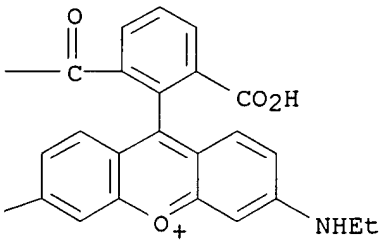


IT **143600-87-7P**
RL: PREP (Preparation)
(preparation of, for DNA sequencing by chain termination, nucleoside thiotriphosphates in, for improved band uniformity and accuracy in)
RN 143600-87-7 CAPLUS
CN Xanthylium, 9-[2-[[[3-[4-amino-1,2-dihydro-2-oxo-1-[tetrahydro-5-(3,5,7,7-tetrahydroxy-3,5,7-trioxido-2,4,6-trioxa-3,5,7-triphosphahept-1-yl)-2-furanyl]-5-pyrimidinyl]-2-propynyl]amino]carbonyl]-6-carboxyphenyl]-3,6-bis(ethylamino)-, chloride, (2R-cis)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L9 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1991:627790 CAPLUS
DN 115:227790
TI Spectrally resolvable rhodamine dyes for **nucleic acid** sequence determination
IN Bergot, John B.; Chakerian, Vergine; Connell, Charles R.; Eadie, J. Scott; Fung, Steven; Hershey, Davis N.; Lee, Linda G.; Menchen, Steven M.; Woo, Sam L.
PA Applied Biosystems, Inc., USA
SO PCT Int. Appl., 29 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9105060	A2	19910418	WO 1990-US5565	19900927 <--
	WO 9105060	A3	19910516		
	W: JP				

RW: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE

	US 5366860	A	19941122	US 1989-415050	19890929
	EP 496749	A1	19920805	EP 1990-914874	19900927 <--
	EP 496749	B1	19951206		

R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE

	JP 05502371	T2	19930428	JP 1990-513838	19900927 <--
	JP 2649102	B2	19970903		
	AT 131210	E	19951215	AT 1990-914874	19900927
PRAI	US 1989-415050	A	19890929		
	WO 1990-US5565	W	19900927		

OS MARPAT 115:227790

AB A spectrally resolvable set of rhodamine dyes are provided for use in the chain termination method of **nucleic acid** sequencing. A different rhodamine dye from the group consisting of tetramethylrhodamine, rhodamine X, rhodamine 6G, and rhodamine 110 is attached to the base of each of the dideoxynucleotides used in the sequencing method by way of an alkynylamino linker. Preferably, the labeled dideoxynucleotides are incorporated into the growing DNA chains by Taq DNA polymerase. The preferred 3'-terminal dideoxynucleotides for labeling for use in sequencing are 2',3'-dideoxy-7-deazaadenosine, 2',3'-dideoxycytidine, 2',3'-dideoxy-7-deazainosine, 2',3'-dideoxy-7-deazaguanosine and 2',3'-dideoxyuridine. Use of the labeled dideoxynucleotides in an automated sequencer identified >450 bases of M13 plasmid DNA.

IT **136977-17-8 136977-21-4 136977-25-8 136977-29-2 136977-35-0 136977-41-8 137004-07-0**
RL: ANST (Analytical study)
(as dye for DNA sequencing)

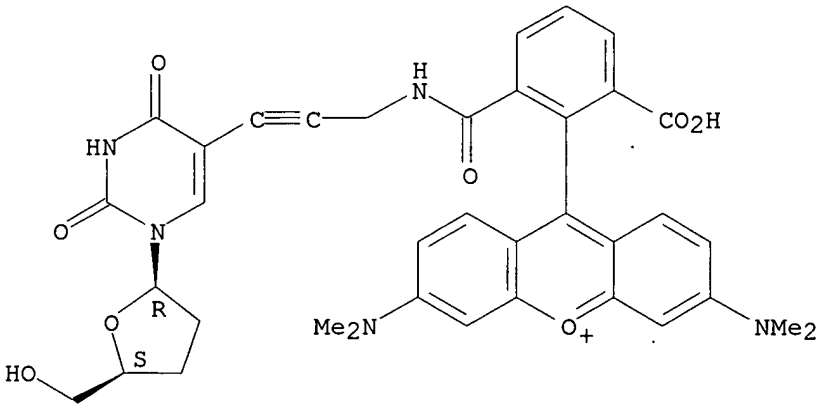
RN 136977-17-8 CAPLUS

CN Xanthylium, 9-[2-carboxy-6-[[[3-[1,2,3,4-tetrahydro-2,4-dioxo-1-[(2R,5S)-tetrahydro-5-(hydroxymethyl)-2-furanyl]-5-pyrimidinyl]-2-propynyl]amino]carbonyl]phenyl]-3,6-bis(dimethylamino)-, acetate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 136977-16-7
CMF C37 H36 N5 O8

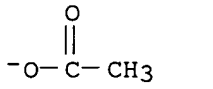
Absolute stereochemistry.



CM 2

CRN 71-50-1

CMF C2 H3 O2

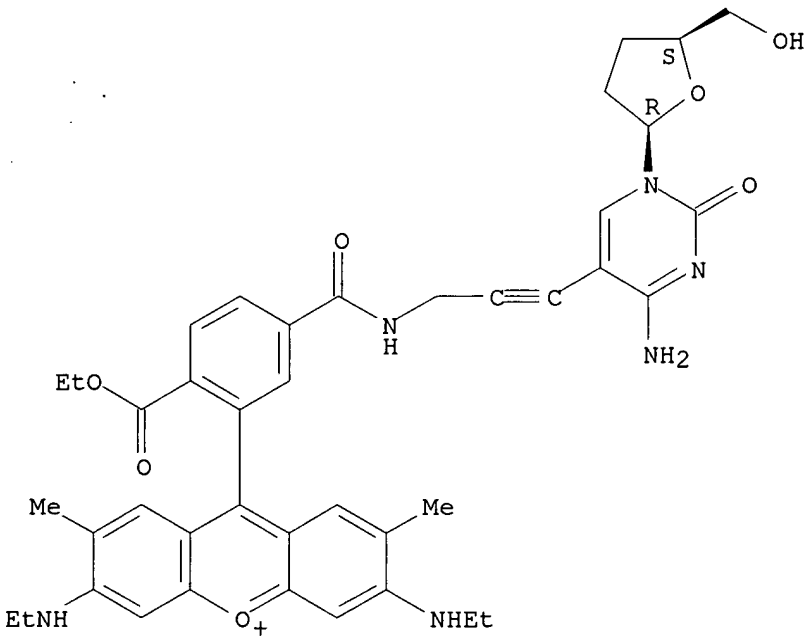


RN 136977-21-4 CAPLUS
CN Xanthylium, 9-[5-[[[3-[4-amino-1,2-dihydro-2-oxo-1-[tetrahydro-5-(hydroxymethyl)-2-furanyl]-5-pyrimidinyl]-2-propynyl]amino]carbonyl]-2-(ethoxycarbonyl)phenyl]-3,6-bis(ethylamino)-2,7-dimethyl-, (2R-cis)-, acetate (salt) (9CI) (CA INDEX NAME)

CM 1

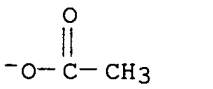
CRN 136977-20-3
CMF C41 H45 N6 O7

Absolute stereochemistry.



CM 2

CRN 71-50-1
CMF C2 H3 O2



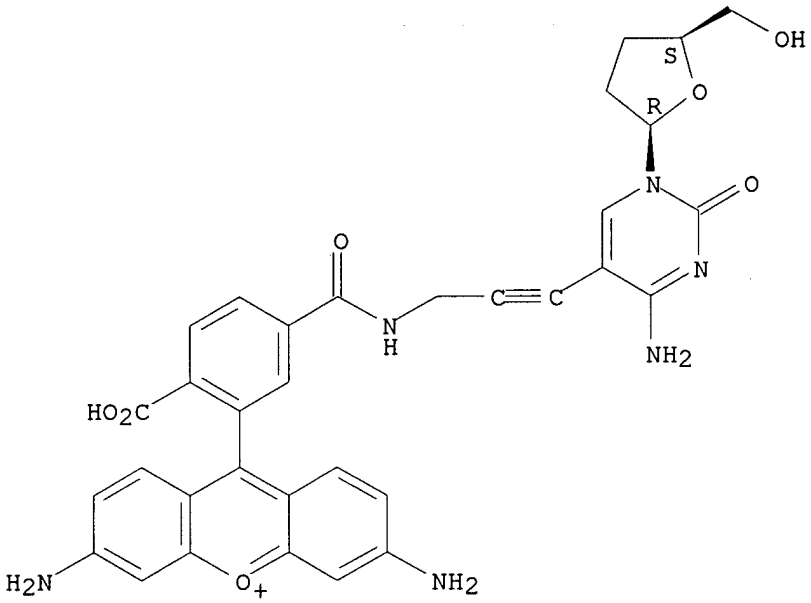
RN 136977-25-8 CAPLUS
CN Xanthylium, 3,6-diamino-9-[5-[[[3-[6-amino-1,2-dihydro-2-oxo-3-[(2R,5s)-tetrahydro-5-(hydroxymethyl)-2-furanyl]-5-pyrimidinyl]-2-

propynyl]amino]carbonyl]-2-carboxyphenyl]-, acetate (salt) (9CI) (CA INDEX NAME)

CM 1

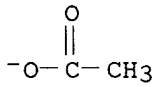
CRN 136977-24-7
CMF C33 H29 N6 O7

Absolute stereochemistry.



CM 2

CRN 71-50-1
CMF C2 H3 O2

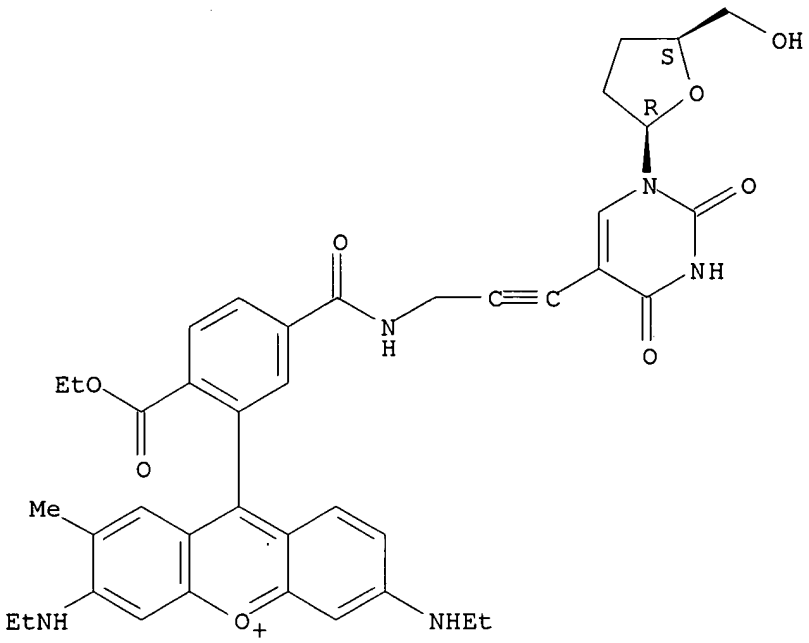


RN 136977-29-2 CAPLUS
CN Xanthylium, 9-[2-(ethoxycarbonyl)-5-[[[3-[1,2,3,4-tetrahydro-2,4-dioxo-1-[(2R,5S)-tetrahydro-5-(hydroxymethyl)-2-furanyl]-5-pyrimidinyl]-2-propynyl]amino]carbonyl]phenyl]-3,6-bis(ethylamino)-2-methyl-, acetate (salt) (9CI) (CA INDEX NAME)

CM 1

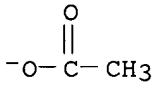
CRN 136977-28-1
CMF C40 H42 N5 O8

Absolute stereochemistry.



CM 2

CRN 71-50-1
CMF C2 H3 O2

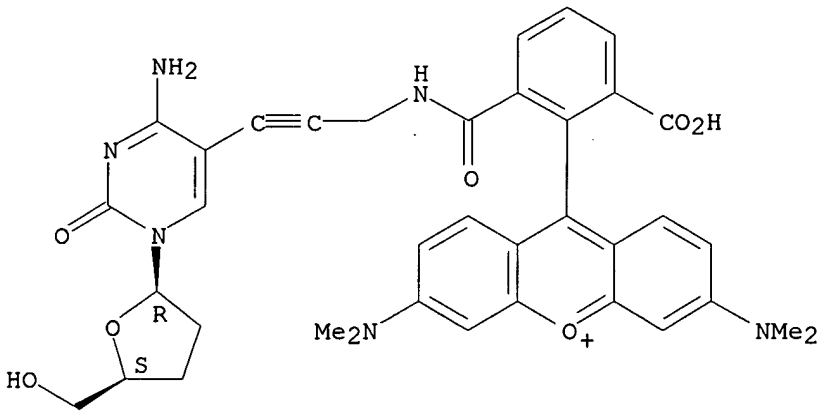


RN 136977-35-0 CAPLUS
CN Xanthylium, 9-[2-[[[3-[4-amino-1,2-dihydro-2-oxo-1-[tetrahydro-5-(hydroxymethyl)-2-furanyl]-5-pyrimidinyl]-2-propynyl]amino]carbonyl]-6-carboxyphenyl]-3,6-bis(dimethylamino)-, (2R-cis)-, acetate (salt) (9CI) (CA INDEX NAME)

CM 1

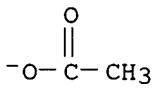
CRN 136977-34-9
CMF C37 H37 N6 O7

Absolute stereochemistry.



CM 2

CRN 71-50-1
CMF C2 H3 O2

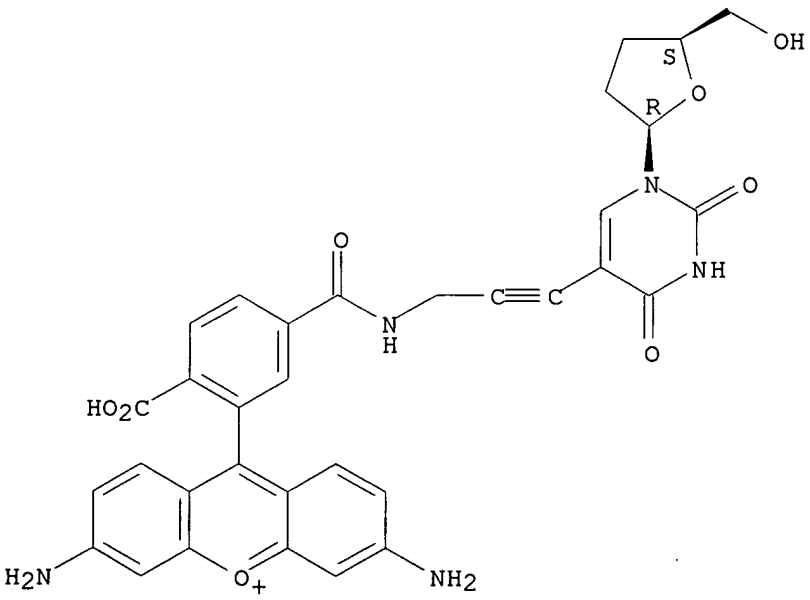


RN 136977-41-8 CAPLUS
CN Xanthylium, 3,6-diamino-9-[2-carboxy-5-[[[3-[1,2,3,4-tetrahydro-2,4-dioxo-1-[(2R,5S)-tetrahydro-5-(hydroxymethyl)-2-furanyl]-5-pyrimidinyl]-2-propynyl]amino]carbonyl]phenyl]-, acetate (salt) (9CI) (CA INDEX NAME)

CM 1

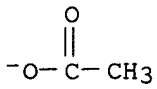
CRN 136977-40-7
CMF C33 H28 N5 O8

Absolute stereochemistry.



CM 2

CRN 71-50-1
CMF C2 H3 O2

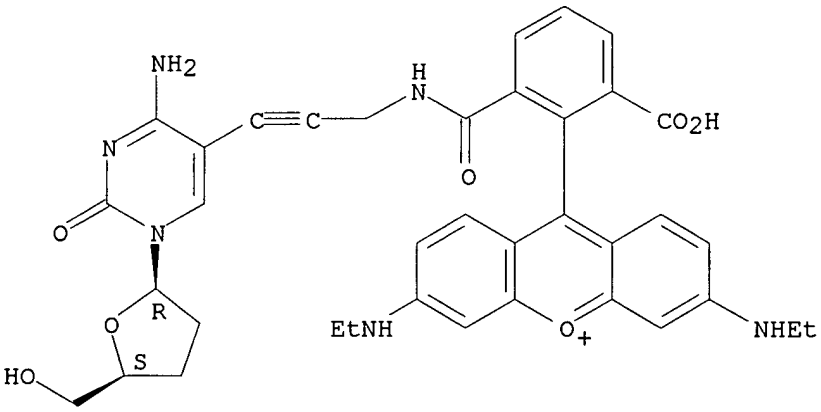


RN 137004-07-0 CAPLUS
CN Xanthylium, 9-[2-[[[3-[4-amino-1,2-dihydro-2-oxo-1-[tetrahydro-5-(hydroxymethyl)-2-furanyl]-5-pyrimidinyl]-2-propynyl]amino]carbonyl]-6-carboxyphenyl]-3,6-bis(ethylamino)-, (2R-cis)-, acetate (salt) (9CI) (CA INDEX NAME)

CM 1

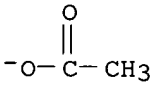
CRN 137004-06-9
CMF C37 H37 N6 O7

Absolute stereochemistry.



CM 2

CRN 71-50-1
CMF C2 H3 O2

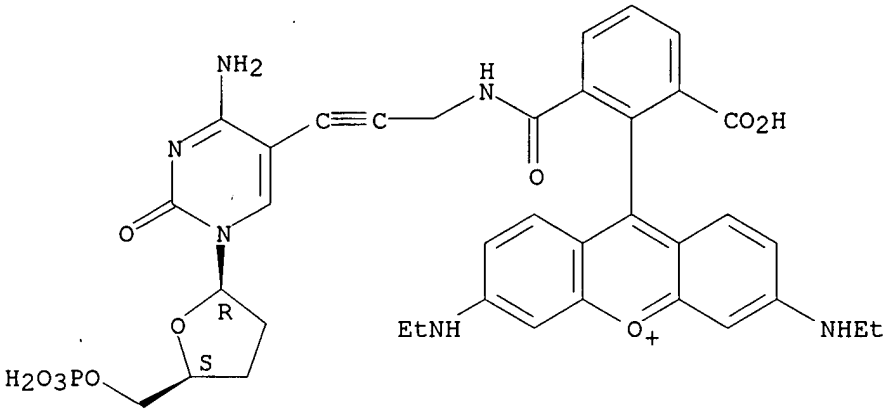


IT **136977-52-1P 136977-55-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as dye for DNA sequencing)
RN 136977-52-1 CAPLUS
CN Xanthylium, 9-[2-[[[3-[4-amino-1,2-dihydro-2-oxo-1-[tetrahydro-5-[(phosphonooxy)methyl]-2-furanyl]-5-pyrimidinyl]-2-propynyl]amino]carbonyl]-6-carboxyphenyl]-3,6-bis(ethylamino)-, (2R-cis)-, acetate (9CI) (CA INDEX NAME)

CM 1

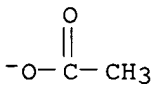
CRN 136977-51-0
CMF C37 H38 N6 O10 P

Absolute stereochemistry.



CM 2

CRN 71-50-1
CMF C2 H3 O2

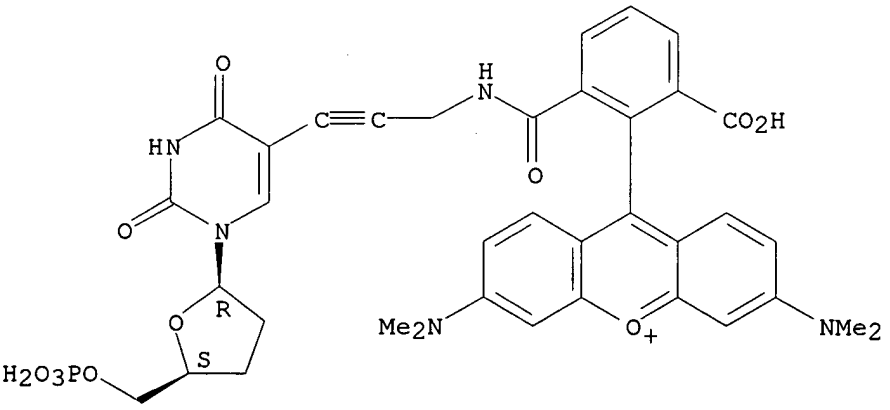


RN 136977-55-4 CAPLUS
CN Xanthylium, 9-[2-carboxy-6-[[[3-[1,2,3,4-tetrahydro-2,4-dioxo-1-[tetrahydro-5-[(phosphonooxy)methyl]-2-furanyl]-5-pyrimidinyl]-2-propynyl]amino]carbonyl]phenyl]-3,6-bis(dimethylamino)-, (2R-cis)-, acetate (9CI) (CA INDEX NAME)

CM 1

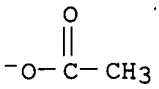
CRN 136977-54-3
CMF C37 H37 N5 O11 P

Absolute stereochemistry.

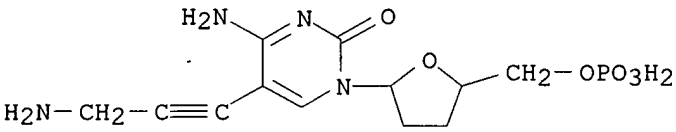


CM 2

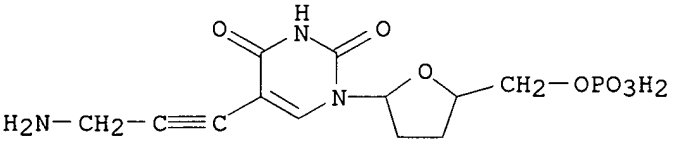
CRN 71-50-1
CMF C2 H3 O2



IT **136977-58-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with rhodamine X ester)
RN 136977-58-7 CAPLUS
CN 5'-Cytidylic acid, 5-(3-amino-1-propynyl)-2',3'-dideoxy- (9CI) (CA INDEX NAME)



IT **136977-56-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with tetramethylrhodamine ester)
RN 136977-56-5 CAPLUS
CN 5'-Uridylic acid, 5-(3-amino-1-propynyl)-2',3'-dideoxy- (9CI) (CA INDEX NAME)



L9 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1991:409259 CAPLUS
DN 115:9259
TI Preparation of crosslinking oligonucleotides as **nucleic acid** hybridization probes
IN Petrie, Charles R.; Meyer, Richard B.; Tabone, John C.; Hurst, Gerald D.
PA Microprobe Corp., USA
SO PCT Int. Appl., 42 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 8

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9014353	A1	19901129	WO 1990-US2740	19900515 <--
	W: CA, JP				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE				
	EP 472648	A1	19920304	EP 1990-908844	19900515 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE				

	JP 04507402	T2	19921224	JP 1990-508242	19900515 <--
	US 5824796	A	19981020	US 1994-334490	19941104
	US 38416	E	20040203	US 2000-693213	20001019
PRAI	US 1989-353857	A	19890518		
	US 1988-250474	B2	19880928		
	WO 1990-US2740	W	19900515		
	US 1993-49807	B1	19930420		
	US 1994-334490	A5	19941104		

OS MARPAT 115:9259

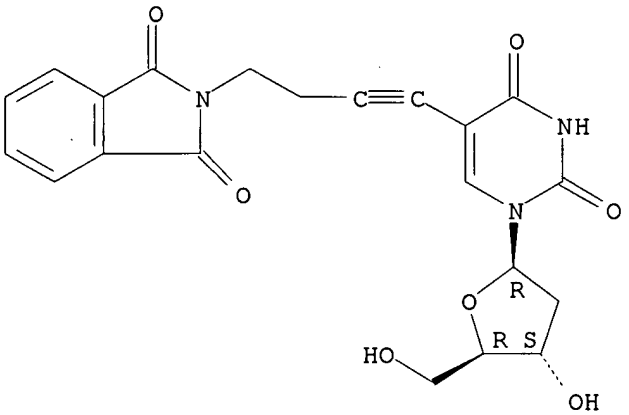
AB R1-B-(CH2)q-Yr-(CH2)m-A1 [R1 = H, sugar (analog) moiety optionally containing Q1, Q2, Q3, P, etc.; Q1 = OH, OP(O)(OH)2, OP(O)(OH)OP(O)(OH)2; Q2 = O, S; Q3 = CH2R2, SR2, OR2, NR2R3; R2, R3 = H, alkyl; B = **nucleic acid** base or an analog thereof; Y = functional linking group; m, q = 0, 1-8 integer; r = 0, 1; A1 = leaving group], useful as **nucleic acid** hybridization probes and therefore useful for diagnosis of diseases, were prepared Reaction of 5-iodo-2'-deoxyuridine in DMF with 4-phthalimido-1-butyne in the presence of (Ph3P)4Pd and Et3N at 60° for 3 h gave 5-(4-phthalimido-1-butyn-1-yl)-2'-deoxyuridine, whose hydrogenation over Raney Ni gave 5-(4-phthalimidobutyl)-2'-deoxyuridine. 5-[3-(Trifluoroacetamido)propyl]-2'-deoxyuridine was prepared similarly and converted according to known methods into 5'-O-(dimethoxytrityl)-2'-deoxyuridine-3'-(N,N-diisopropyl)phosphoramidite cyanoethyl ester, which was used in the automated synthesis of 3'-CT TCC U1TG TAG CTG-5' [I; U1 = 5-(3-aminopropyl)-2'-deoxyuridine residue]. This was reacted with N-(iodoactoxy)succinimide to give II [U1 = 5-(3-iodoacetamidopropyl)-2'-uridine residue], whose crosslinking to a 30-mer oligonucleotide derived from human papillomavirus (HPV) was evaluated.

IT **134140-85-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenation of)

RN 134140-85-5 CAPLUS

CN Uridine, 2'-deoxy-5-[4-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)-1-butynyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L9 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1990:631903 CAPLUS

DN 113:231903

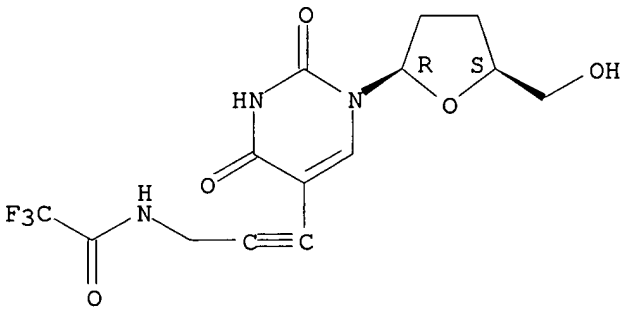
TI **Nucleic acid** related compounds. 59. Solvent, not palladium oxidation state, is the primary determinant for successful coupling of terminal alkynes with iodonucleosides

AU Robins, Morris J.; Vinayak, Ravi S.; Wood, Steven G.

CS Dep. Chem., Brigham Young Univ., Provo, UT, 84602, USA

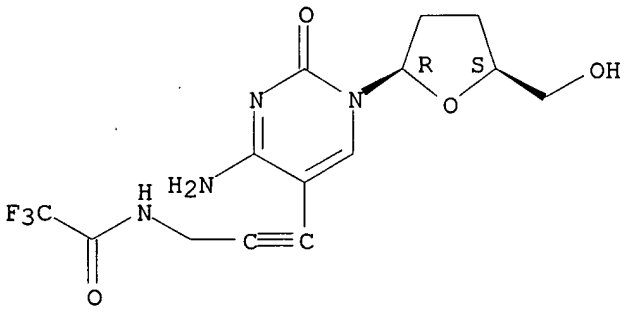
SO Tetrahedron Letters (**1990**), 31(26), 3731-4
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 113:231903
AB Coupling of iodo nucleosides with terminal alkynes such as 3-(acylamino)propynes, whose initial products readily undergo secondary cyclization reactions, can be effected smoothly by the standard catalysis with Pd(PPh3)4 or (Ph3P)2PdCl2/CuI/Et3N in DMF.
IT **114748-60-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 114748-60-6 CAPLUS
CN Uridine, 2',3'-dideoxy-5-[3-[(trifluoroacetyl)amino]-1-propynyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



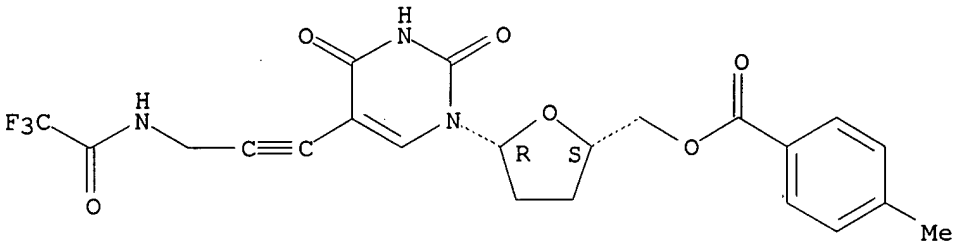
IT **114748-58-2P 130532-28-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by alkynylation of iodo analog, DMF as solvent in)
RN 114748-58-2 CAPLUS
CN Cytidine, 2',3'-dideoxy-5-[3-[(trifluoroacetyl)amino]-1-propynyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

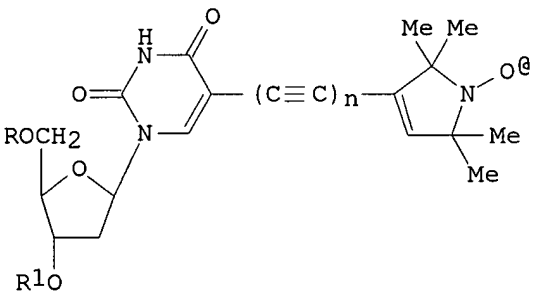


RN 130532-28-4 CAPLUS
CN Benzoic acid, 4-methyl-, [tetrahydro-5-[4-hydroxy-2-oxo-5-[3-[(trifluoroacetyl)amino]-1-propynyl]-1(2H)-pyrimidinyl]-2-furanyl]methyl ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



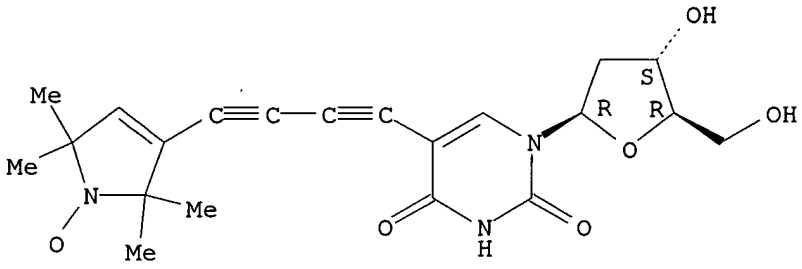
L9 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:515768 CAPLUS
DN 113:115768
TI DNA dynamics from a spin probe: dependence of probe motion on tether length
AU Kirchner, James J.; Hustedt, Eric J.; Robinson, Bruce H.; Hopkins, Paul B.
CS Dep. Chem., Univ. Washington, Seattle, WA, 98195, USA
SO Tetrahedron Letters (**1990**), 31(5), 593-6
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 113:115768
GI



I

AB The phosphoramidite I [R = C(C6H4OMe-p)2Ph, R1 = P(OCH2CH2CN)N(CHMe2), n = 2] (II) a spin labeled analog of thymidine, was synthesized and incorporated into the deoxyoligonucleotide 5'-d(CGCGAATT*CGCG) (T* = spin-labeled phosphoramidite II). This substance adopts a duplex structure, as shown by gel electrophoretic mobility. The ESR spectrum of the spin labeled duplex in solution was indicative of subnanosecond probe motion, a result which contrasts with the ca. 5 ns correlation time determined for the corresponding analog I (n = 1) (III). Steric inhibition of rotation of the nitroxide-bearing ring of III not present in **nucleic acid** containing II accounts for this difference.
IT **129077-26-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dimethoxytritylation and phosphitylation of)
RN 129077-26-5 CAPLUS
CN 1H-Pyrrol-1-yloxy, 3-[4-[1-(2-deoxy-β-D-erythro-pentofuranosyl)-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]-1,3-butadiynyl]-2,5-dihydro-2,2,5,5-tetramethyl- (9CI) (CA INDEX NAME)

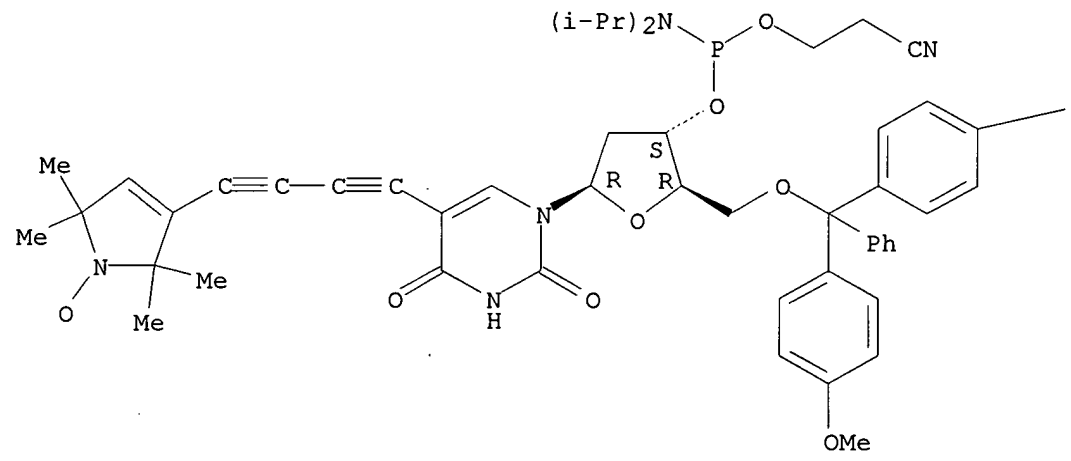
Absolute stereochemistry.



IT **129077-27-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and incorporation of, into deoxyoligonucleotide, in study of DNA dynamics)
RN 129077-27-6 CAPLUS
CN 1H-Pyrrol-1-yloxy, 3-[4-[1-[5-O-[bis(4-methoxyphenyl)phenylmethyl]-3-O-[[bis(1-methylethyl)amino](2-cyanoethoxy)phosphino]-2-deoxy-β-D-erythro-pentofuranosyl]-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]-1,3-butadiynyl]-2,5-dihydro-2,2,5,5-tetramethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

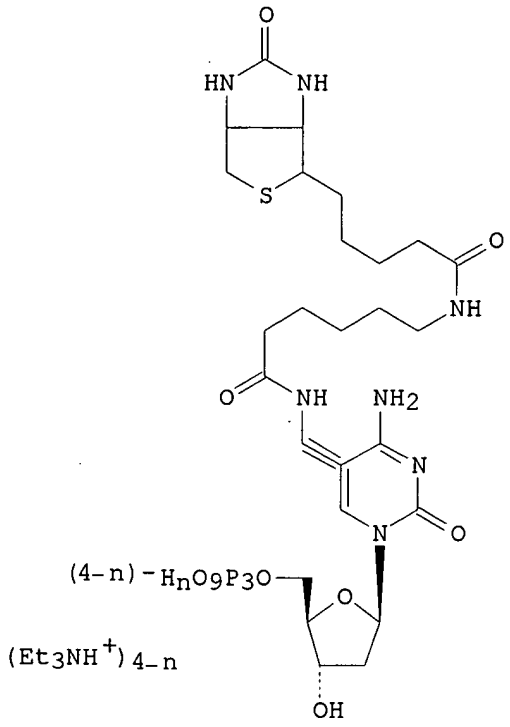
—OMe

L9 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:213554 CAPLUS
DN 112:213554
TI Mobility-shifting analog for differentiation of **nucleic acid** segments on the basis of nucleotide differences
IN Kornher, John S.; Livak, Kenneth J.
PA du Pont de Nemours, E. I., and Co., USA
SO U.S., 10 pp.
CODEN: USXXAM
DT Patent
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4879214	A	19891107	US 1988-272068	19881115 <--
	EP 369360	A2	19900523	EP 1989-120944	19891111 <--
	EP 369360	A3	19910109		
	R: BE, DE, FR, GB, IT, NL, SE				
	DK 8905699	A	19900516	DK 1989-5699	19891114 <--
	JP 02231099	A2	19900913	JP 1989-294099	19891114 <--
	CA 2003038	AA	19900515	CA 1989-2003038	19891115 <--
PRAI	US 1988-272068	A	19881115		

GI



I

AB A process for distinguishing **nucleic acid** segments on the basis of nucleotide differences comprises (1) synthesizing complementary **nucleic acid** strands on each of ≥2 target **nucleic acid** templates with a **nucleic acid** polymerase and nucleoside triphosphate substrates, where ≥1 of the natural nucleoside triphosphate substrates is completely replaced by a mobility-shifting analog; (2) if necessary, denaturing the synthesized strands from the templates; and (3) comparing the mobility of the sep. synthesized strands in a single-stranded form with a size-fractionation medium. Thus, the mobility shifting analog I was synthesized from 5-(3-amino-1-propynyl)-2'-deoxycytidine-5'-triphosphate (preparation given) and Na sulfosuccinimidyl 6-(biotinamido)hexanoate. I was used in primer extension anal. to compare segments of 2 alleles of the human insulin receptor gene differing by a single nucleotide substitution. Polymerase chain reactions were used to amplify a 140-base pair region of DNA encoding the above receptor from 2 individuals, 1 homozygous and 1 heterozygous for deoxycytidine at position 2143. The amplified templates were hybridized with a 20-base pair primer.

A primer extension reaction was then performed, using dATP, dGTP, dUTP, and I or dCTP as substrate. Electrophoretic separation of the primer extension products demonstrated electrophoretic mobility shifts when I was substituted for dCTP in the extension reaction. Incorporation of I allowed for the discrimination of 2 templates from the same individual that differed by a single deoxycytidine substitution.

IT **126786-05-8**
RL: ANST (Analytical study)
(as mobility-shifting analog, **nucleic acid** differentiation using primer extension reaction with)

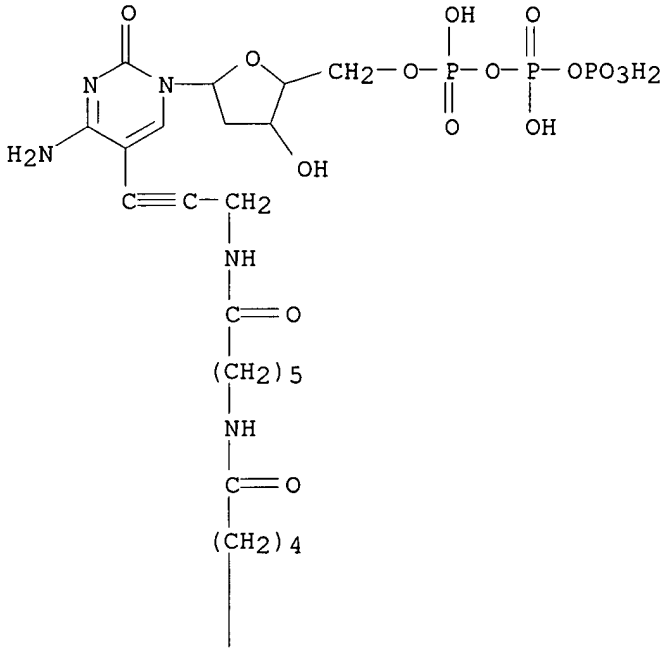
RN 126786-05-8 CAPLUS

CN Cytidine 5'-(tetrahydrogen triphosphate), 2'-deoxy-5-[3-[[6-[[5-(hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl)-1-oxopentyl]amino]-1-oxohexyl]amino]-1-propynyl]-, [3aS-(3aα,4β,6aα)]-, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

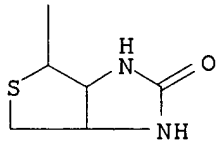
CM 1

CRN 124607-57-4
CMF C28 H44 N7 O16 P3 S

PAGE 1-A

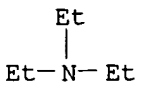


PAGE 2-A



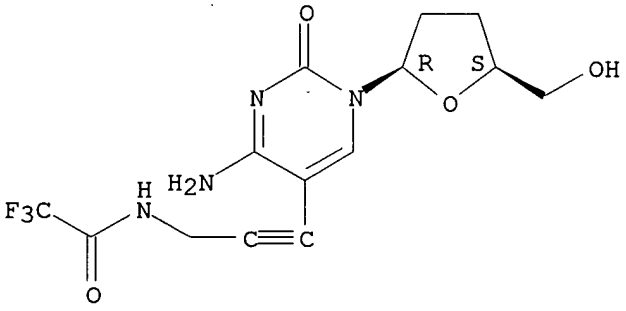
CM 2

CRN 121-44-8
CMF C6 H15 N



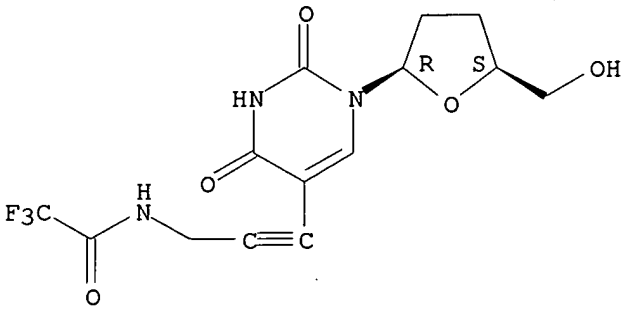
L9 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1989:574570 CAPLUS
DN 111:174570
TI Palladium-catalyzed synthesis of alkynylamino nucleosides. A universal linker for nucleic acids
AU Hobbs, Frank W., Jr.
CS Cent. Res. Dev. Dep., E. I. Dupont de Nemours and Co., Wilmington, DE, 19898, USA
SO Journal of Organic Chemistry (**1989**), 54(14), 3420-2
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 111:174570
AB A method for attaching alkynylamino linkers to nucleosides and nucleotides is described. Protected or unprotected alkynylamines are coupled to iodo nucleosides in DMF using Pd(PPh3)4-CuI (1:2), a catalyst system superior to the standard Pd(II) species. The resulting alkynylamino nucleosides are useful for enzymic or chemical labeling of all four bases of DNA.
IT **114748-58-2P 114748-60-6P 115899-38-2P**
115899-40-6P 115899-42-8P 115899-44-0P
115899-45-1P 115899-46-2P 120609-05-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 114748-58-2 CAPLUS
CN Cytidine, 2',3'-dideoxy-5-[3-[(trifluoroacetyl)amino]-1-propynyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



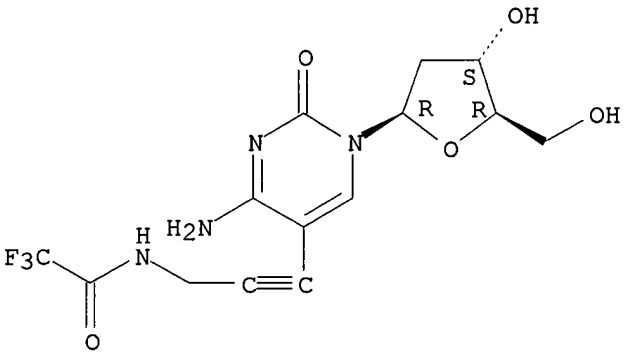
RN 114748-60-6 CAPLUS
CN Uridine, 2',3'-dideoxy-5-[3-[(trifluoroacetyl)amino]-1-propynyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



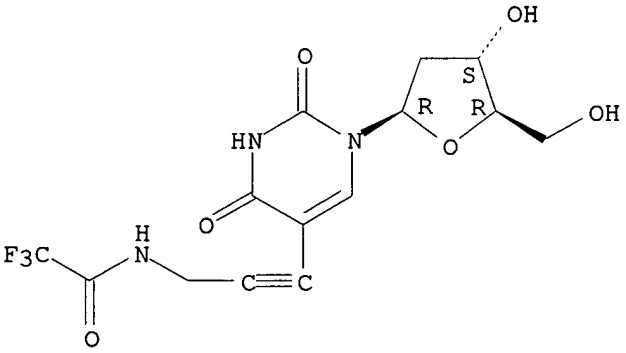
RN 115899-38-2 CAPLUS
CN Cytidine, 2'-deoxy-5-[3-[(trifluoroacetyl)amino]-1-propynyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

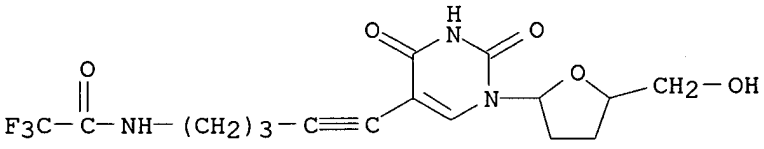


RN 115899-40-6 CAPLUS
CN Uridine, 2'-deoxy-5-[3-[(trifluoroacetyl)amino]-1-propynyl]- (9CI) (CA INDEX NAME)

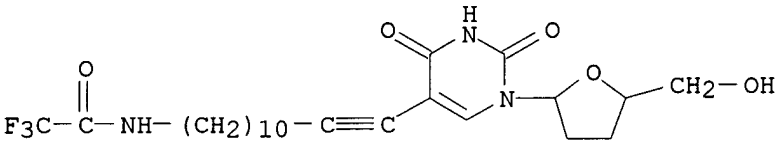
Absolute stereochemistry.



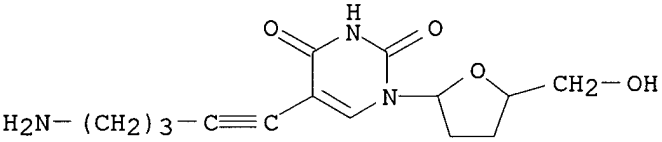
RN 115899-42-8 CAPLUS
CN Uridine, 2',3'-dideoxy-5-[5-[(trifluoroacetyl)amino]-1-pentynyl]- (9CI) (CA INDEX NAME)



RN 115899-44-0 CAPLUS
CN Uridine, 2',3'-dideoxy-5-[12-[(trifluoroacetyl)amino]-1-dodecynyl]- (9CI) (CA INDEX NAME)

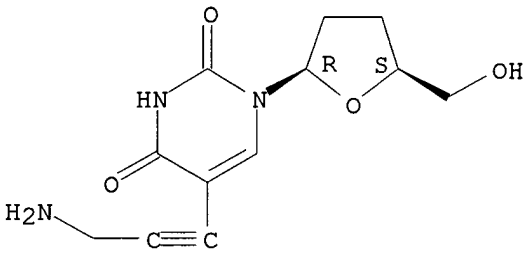


RN 115899-45-1 CAPLUS
CN Uridine, 5-(5-amino-1-pentynyl)-2',3'-dideoxy- (9CI) (CA INDEX NAME)



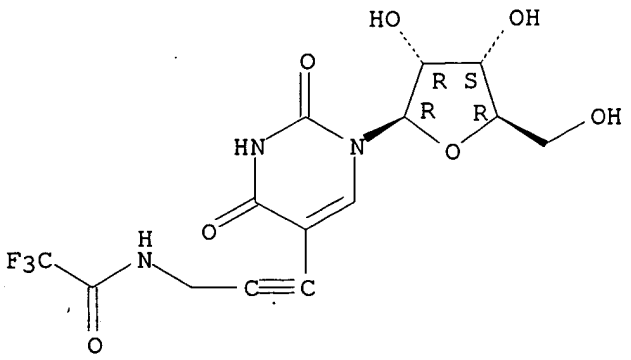
RN 115899-46-2 CAPLUS
CN Uridine, 5-(3-amino-1-propynyl)-2',3'-dideoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 120609-05-4 CAPLUS
CN Uridine, 5-[3-[(trifluoroacetyl)amino]-1-propynyl]- (9CI) (CA INDEX NAME)

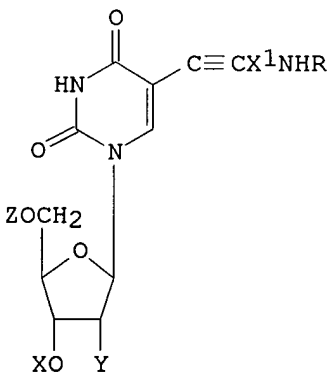
Absolute stereochemistry.



L9 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1989:439836 CAPLUS
DN 111:39836
TI Preparation of 5-(3-aminoprop-1-ynyl)deoxyuridine derivatives and their use for synthesis of DNA and RNA labeled with nonradioactive markers.
IN Haralambidis, Jim
PA Florey, Howard, Institute of Experimental Physiology and Medicine, Australia
SO PCT Int. Appl., 58 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 8810264	A1	19881229	WO 1988-AU207	19880624 <--
	W: AU, JP, US				
	RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
	AU 8819909	A1	19890119	AU 1988-19909	19880624 <--
	AU 598946	B2	19900705		
	EP 366685	A1	19900509	EP 1988-905594	19880624 <--
	EP 366685	B1	19941019		
	R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
	JP 02504144	T2	19901129	JP 1988-505657	19880624 <--
	JP 2828642	B2	19981125		
	CA 1340032	A1	19980908	CA 1988-570427	19880624
PRAI	AU 1987-2666	A	19870624		
	WO 1988-AU207	A	19880624		

OS MARPAT 111:39836
GI



I

AB The title nucleoside derivs. [I; Y = H, (un)protected OH; X = H, phosphonate group, P(OQ)NR1R2; R1, R2 = (un)branched, (un)substituted alkyl; Q = phosphate protecting group; Z = H, phosphate, triphosphate group; X1 = (un)branched (1-15 alkyl; R = amino protecting group, A, Y1NHA; A = fluorophore (e.g. fluorescein) or other non-radioactive detectable group (e.g. biotin, avidin, colloidal Au or Ag, ferritin, and enzymes such as β-galactosidase, urease, peroxidase); γ1 = (un)branched C1-10 alkylcarbonyl], useful for preparing DNA and RNA labeled with non-radioactive detectable markers as **nucleic acid** hybridization probes, were prepared Thus, coupling of 3',5'-di-O-p-toluoyl-5-iododeoxyuridine with BOCNHCH2C.tplbond.CH (BOC = CO2CMe3) in EtOAc in the presence of (Ph3P)2PdCl2, CuI and Et3N gave 84% I (Y = H, Z = X = toluoyl, X1NHR = C .tplbond. CCH2NHGBOC). Saponification of the latter with K2CO3 in MeOH followed by reaction with 4,4'-dimethoxytrityl chloride (DMTrCl) in pyridine gave 68% I (X = Y = H, Z = DMTr, X1NHR = C.tplbond.CCH2NHBOC) which was treated with [(Me2CH)2N]2POMe in CH2Cl2 containing tetrazole and (Me2CH)2NH to give I [Y = H, Z = CMTr, X = P(OMe)N(CHMe2)2, X1NHR = C.tplbond.CCH2NHBOC]. The latter can be reacted by the phosphoramidite method to prepare oligonucleotides which incorporate the modified nucleoside on the 5'-end or internally.

IT **114079-33-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acylation of, with nitrophenylaminohexanoate derivative)

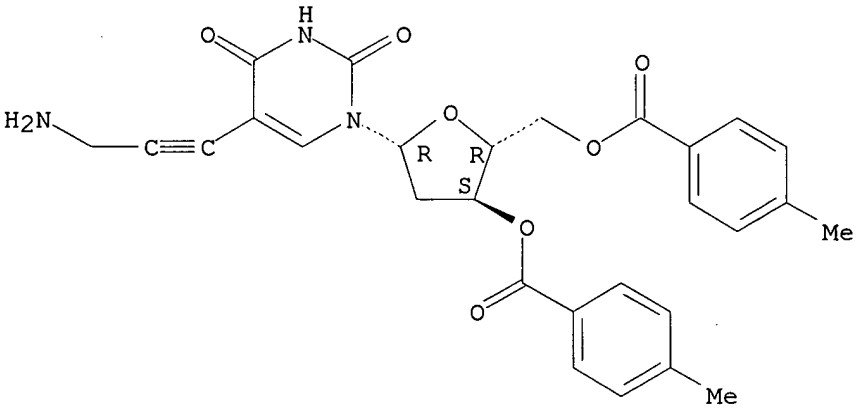
RN 114079-33-3 CAPLUS

CN Uridine, 5-(3-amino-1-propynyl)-2'-deoxy-, 3',5'-bis(4-methylbenzoate), mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

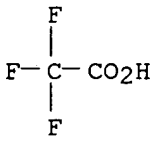
CRN 114079-32-2
CMF C28 H27 N3 O7

Absolute stereochemistry.



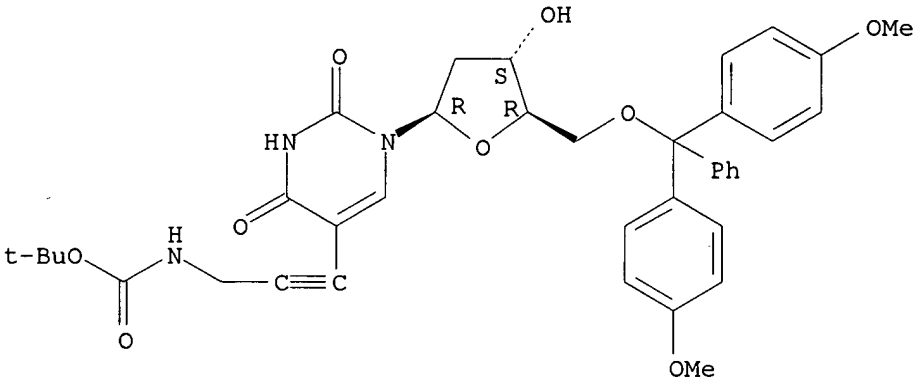
CM 2

CRN 76-05-1
CMF C2 H F3 O2



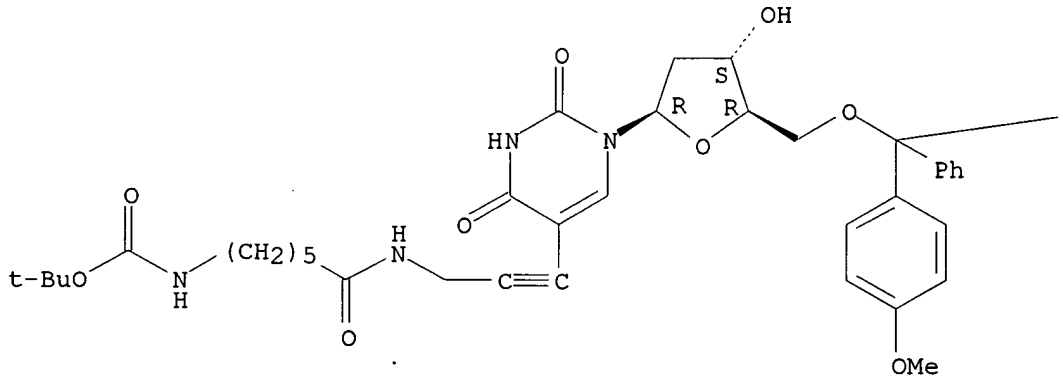
IT **114079-31-1P 114079-35-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation of, with bis(diisopropylamino)methoxyphosphine
)
RN 114079-31-1 CAPLUS
CN Carbamic acid, [3-[1-[5-O-[bis(4-methoxyphenyl)phenylmethyl]-2-deoxy-β-D-erythro-pentofuranosyl]-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]-2-propynyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

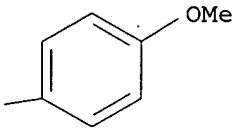
Absolute stereochemistry.



RN 114079-35-5 CAPLUS
CN Carbamic acid, [6-[[3-[1-[5-O-[bis(4-methoxyphenyl)phenylmethyl]-2-deoxy-β-D-erythro-pentofuranosyl]-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]-2-propynyl]amino]-6-oxohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

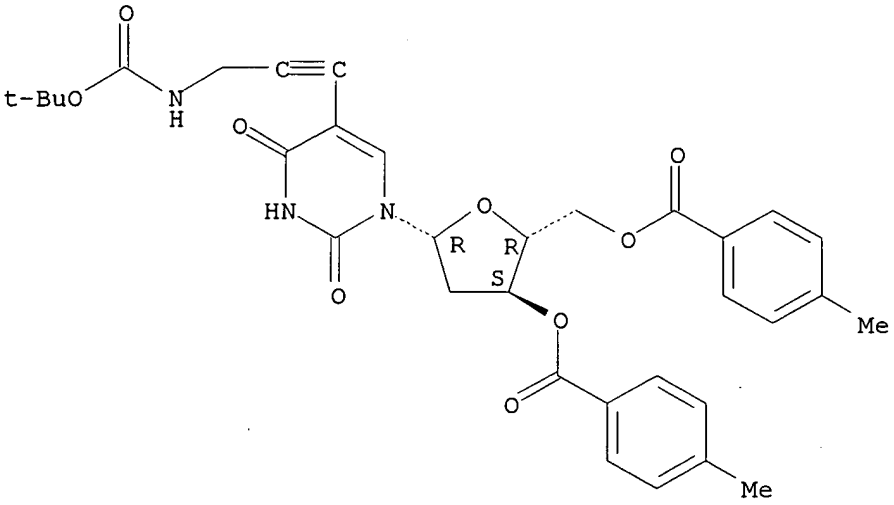
Absolute stereochemistry.





IT **114079-29-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of **nucleic acid** marker)
RN 114079-29-7 CAPLUS
CN Carbamic acid, [3-[1-[2-deoxy-3,5-bis-O-(4-methylbenzoyl)-β-D-erythro-pentofuranosyl]-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]-2-propynyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

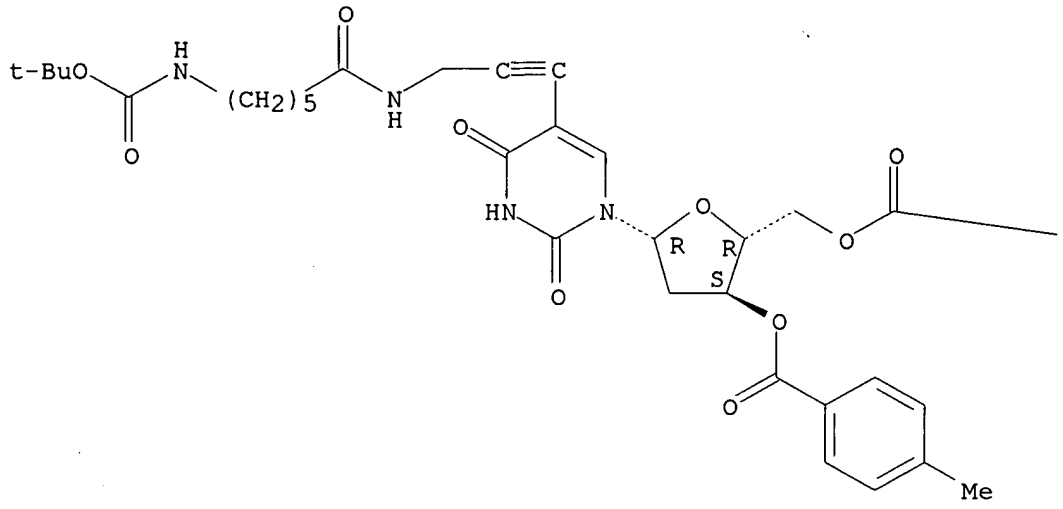
Absolute stereochemistry.



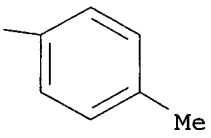
IT **114079-34-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and saponification-alkylation of, by dimethoxytrityl chloride)
RN 114079-34-4 CAPLUS
CN Carbamic acid, [6-[[3-[1-[2-deoxy-3,5-bis-O-(4-methylbenzoyl)-β-D-erythro-pentofuranosyl]-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]-2-propynyl]amino]-6-oxohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



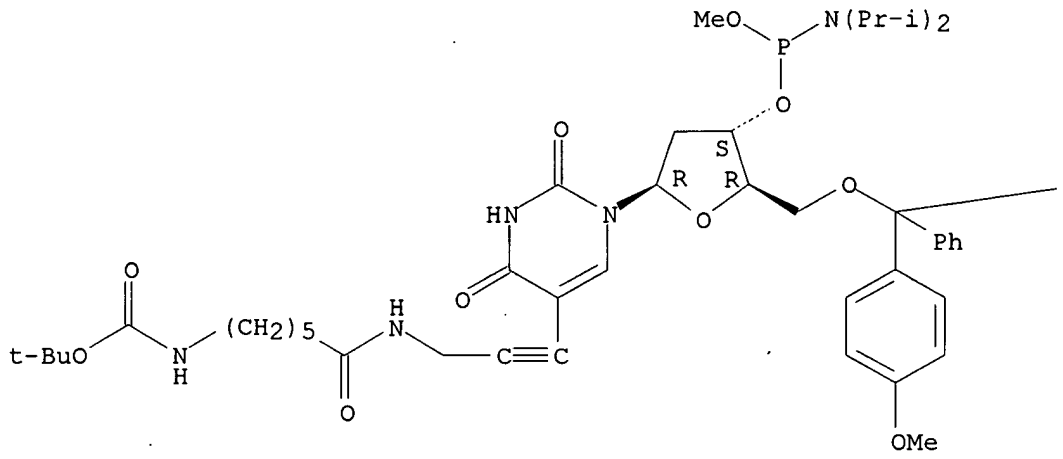
IT **114079-36-6P 114103-42-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for nonradioactive marker-labeled oligonucleotides)

RN 114079-36-6 CAPLUS

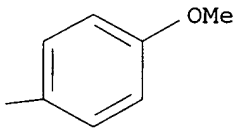
CN Carbamic acid, [6-[[3-[1-[5-O-[bis(4-methoxyphenyl)phenylmethyl]-3-O-[[bis(1-methylethyl)amino]methoxyphosphino]-2-deoxy-β-D-erythro-pentofuranosyl]-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]-2-propynyl]amino]-6-oxohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

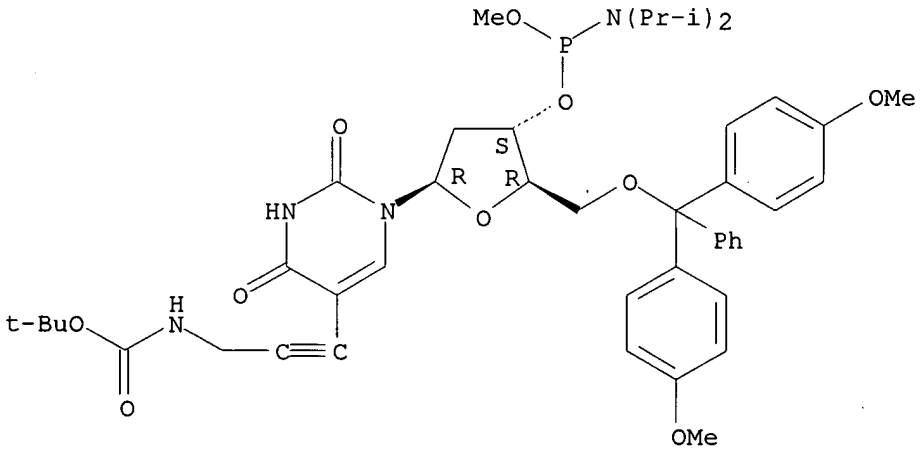


PAGE 1-B



RN 114103-42-3 CAPLUS
CN Carbamic acid, [3-[1-[5-O-[bis(4-methoxyphenyl)phenylmethyl]-3-O-[[bis(1-methylethyl)amino]methoxyphosphino]-2-deoxy-β-D-erythro-pentofuranosyl]-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]-2-propynyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

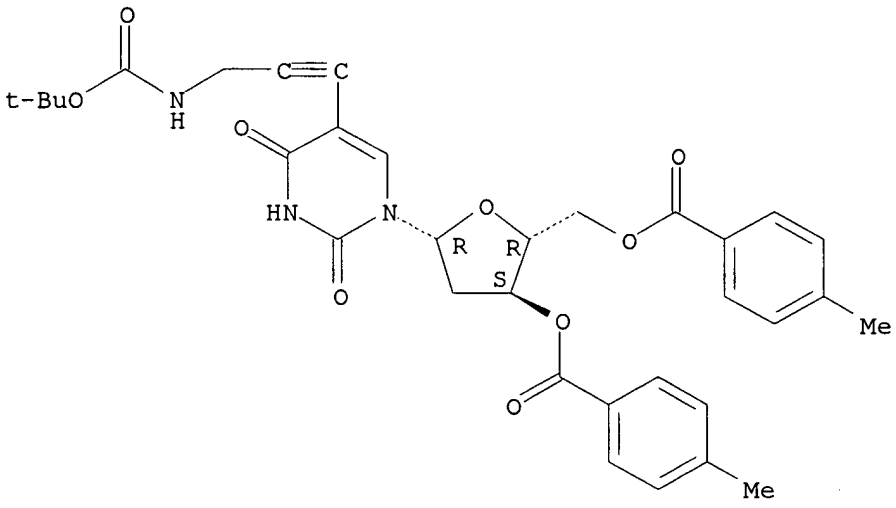
Absolute stereochemistry.



L9 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1988:187182 CAPLUS

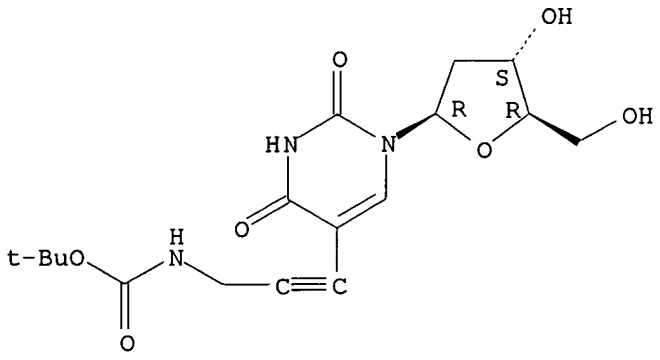
DN 108:187182
TI Preparation of base-modified nucleosides suitable for non-radioactive label attachment and their incorporation into synthetic oligodeoxyribonucleotides
AU Haralambidis, Jim; Chai, Miao; Tregear, Geoffrey W.
CS Howard Florey Inst. Exp. Physiol. Med., Univ. Melbourne, Parkville, 3052, Australia
SO Nucleic Acids Research (**1987**), 15(12), 4857-76
CODEN: NARHAD; ISSN: 0305-1048
DT Journal
LA English
OS CASREACT 108:187182
AB A very mild and efficient procedure has been developed for the preparation of C-5 substituted deoxyuridines. The substituent carries a masked primary aliphatic amino group. These compds. are readily converted into their phosphoramidites and can be used to prepare oligonucleotides carrying one or more aliphatic amino groups. Fluorescein isothiocyanate coupled to these compds. gives oligonucleotide probes carrying multiple fluorescein labels. These compds. have a free 5'-hydroxy group enabling additional 5'- end radioactive labeling for evaluation of their hybridization characteristics. Oligonucleotides carrying a long (11 atom) linker arm to the fluorescein hybridize more efficiently to mRNA than those carrying a short (4 atom) arm. The long linker arm derivs. are comparable to underivatized oligonucleotides in hybridizing to mRNA.
IT **114079-29-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and detoluoylation of)
RN 114079-29-7 CAPLUS
CN Carbamic acid, [3-[1-[2-deoxy-3,5-bis-O-(4-methylbenzoyl)-β-D-erythro-pentofuranosyl]-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]-2-propynyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



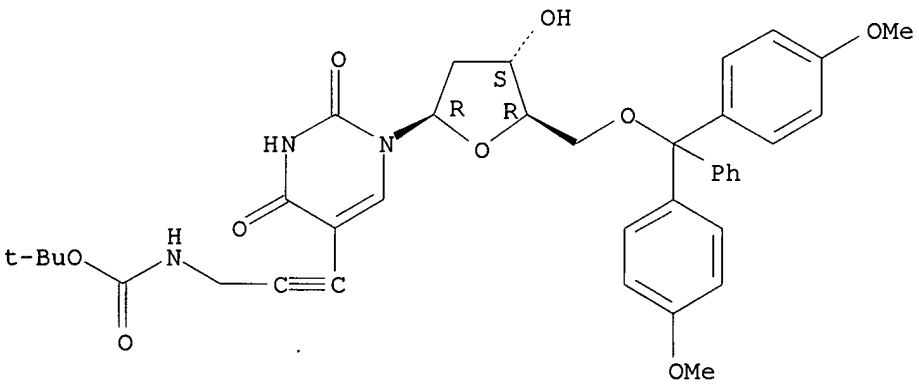
IT **114079-30-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dimethoxytritylation of)
RN 114079-30-0 CAPLUS
CN Carbamic acid, [3-[1-(2-deoxy-β-D-erythro-pentofuranosyl)-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]-2-propynyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **114079-31-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with bis(diisopropylamino)methoxyphosphine)
RN 114079-31-1 CAPLUS
CN Carbamic acid, [3-[1-[5-O-[bis(4-methoxyphenyl)phenylmethyl]-2-deoxy-β-D-erythro-pentofuranosyl]-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]-2-propynyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

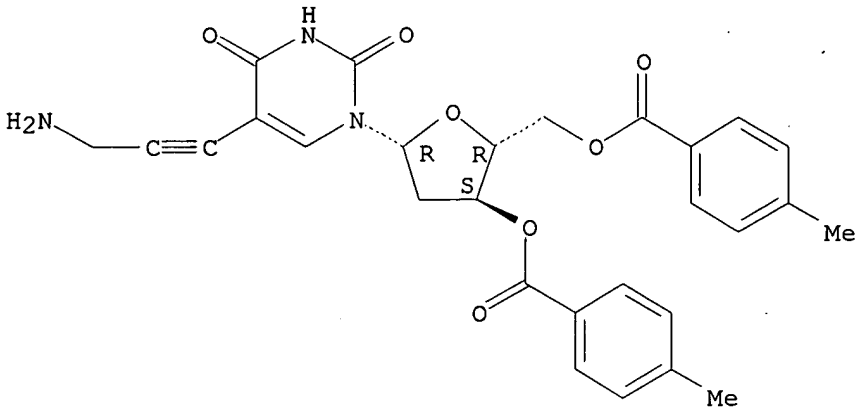


IT **114079-33-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with nitrophenyl aminohexanoate derivative)
RN 114079-33-3 CAPLUS
CN Uridine, 5-(3-amino-1-propynyl)-2'-deoxy-, 3',5'-bis(4-methylbenzoate), mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

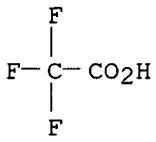
CRN 114079-32-2
CMF C28 H27 N3 O7

Absolute stereochemistry.



CM 2

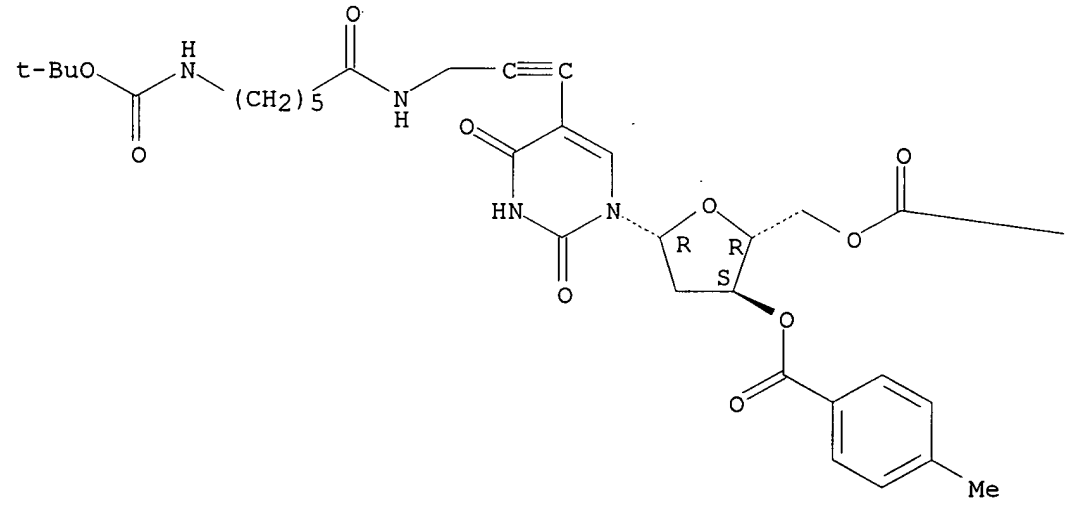
CRN 76-05-1
CMF C2 H F3 O2



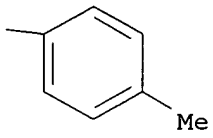
IT **114079-34-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and sequential detoluoylation and dimethoxytritylation of)
RN 114079-34-4 CAPLUS
CN Carbamic acid, [6-[[3-[1-[2-deoxy-3,5-bis-O-(4-methylbenzoyl)-β-D-erythro-pentofuranosyl]-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]-2-propynyl]amino]-6-oxohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



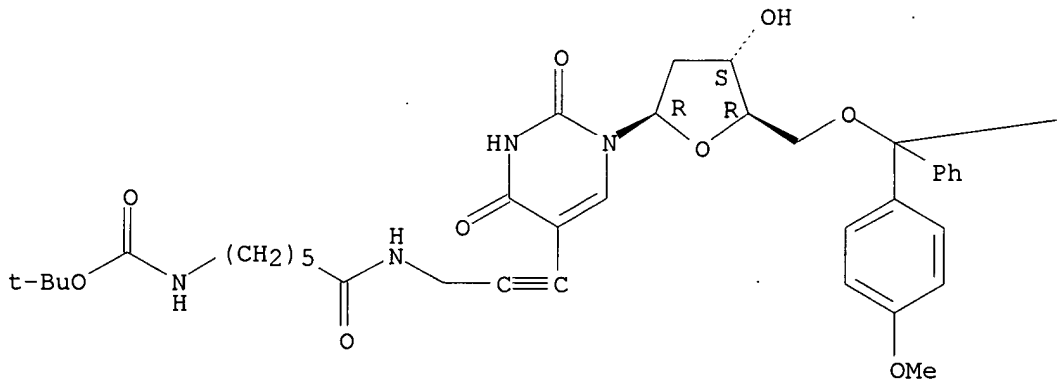
PAGE 1-B



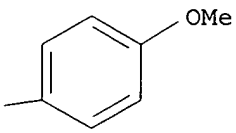
IT **114079-35-5P 114079-36-6P 114103-42-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, intermediate in synthesis of fluorescent-labeled oligodeoxyribonucleotides)
RN 114079-35-5 CAPLUS
CN Carbamic acid, [6-[[3-[1-[5-O-[bis(4-methoxyphenyl)phenylmethyl]-2-deoxy-β-D-erythro-pentofuranosyl]-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]-2-propynyl]amino]-6-oxohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



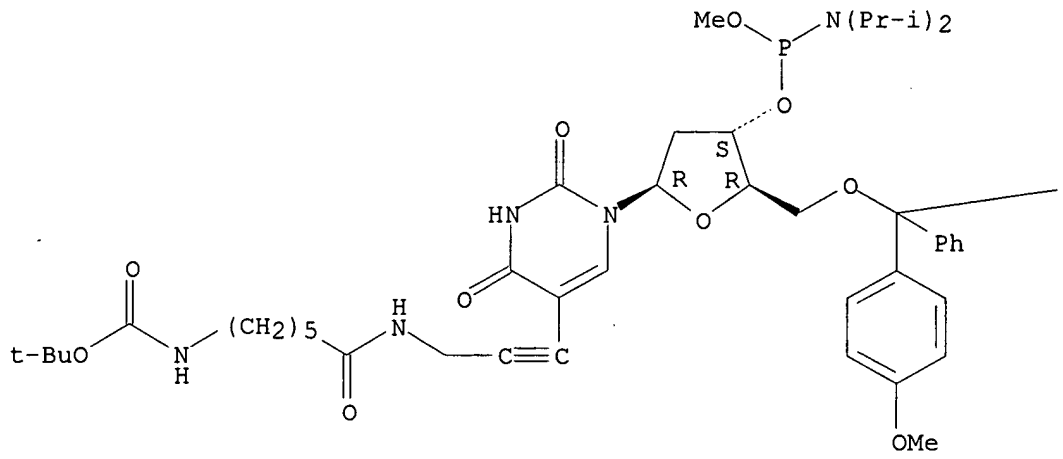
PAGE 1-B



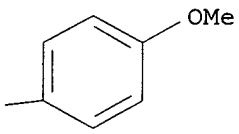
RN 114079-36-6 CAPLUS
CN Carbamic acid, [6-[[3-[1-[5-O-[bis(4-methoxyphenyl)phenylmethyl]-3-O-[[bis(1-methylethyl)amino]methoxyphosphino]-2-deoxy-β-D-erythro-pentofuranosyl]-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]-2-propynyl]amino]-6-oxohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

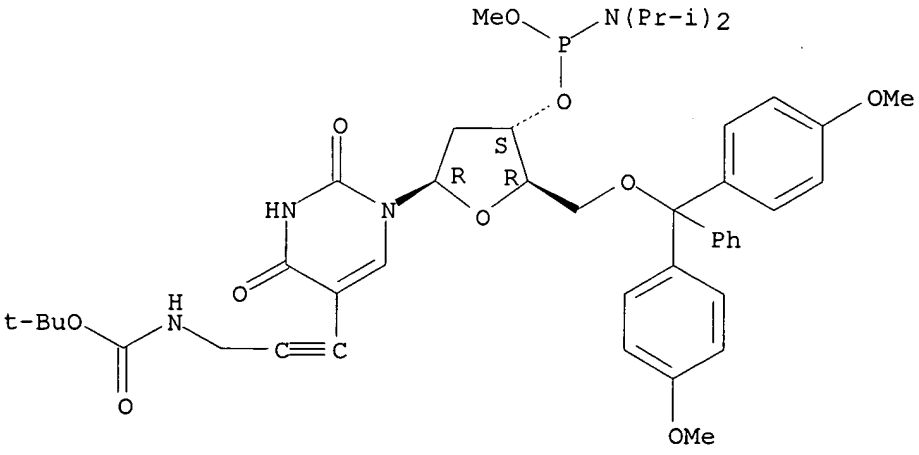


PAGE 1-B



RN 114103-42-3 CAPLUS
CN Carbamic acid, [3-[1-[5-O-[bis(4-methoxyphenyl)phenylmethyl]-3-O-[[bis(1-methylethyl)amino]methoxyphosphino]-2-deoxy-β-D-erythro-pentofuranosyl]-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]-2-propynyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

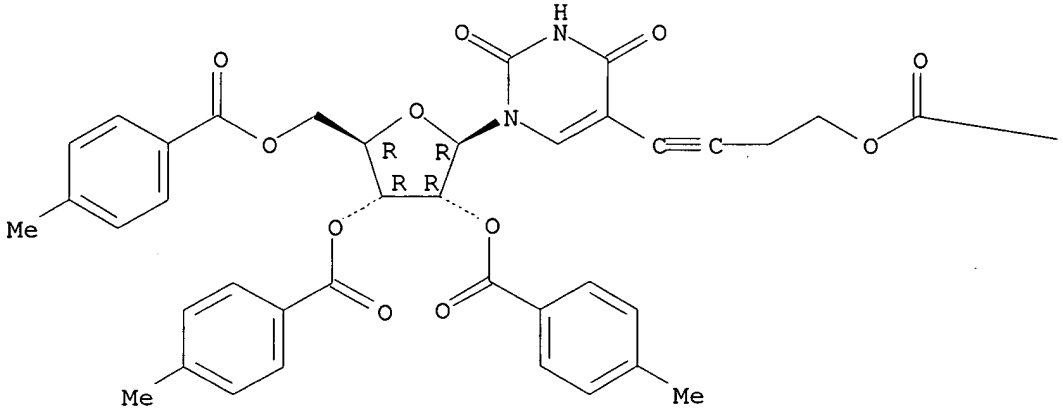
Absolute stereochemistry.

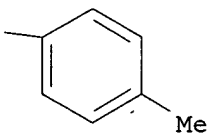


L9 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:215932 CAPLUS
DN 98:215932
TI **Nucleic acid** related compounds. 39. Efficient conversion of 5-iodo to 5-alkynyl and derived 5-substituted uracil bases and nucleosides
AU Robins, Morris J.; Barr, Philip J.
CS Dep. Chem., Univ. Alberta, Edmonton, AB, T6G 2G2, Can.
SO Journal of Organic Chemistry (**1983**), 48(11), 1854-62
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
AB Coupling terminal alkynes with 5-iodo-1-methyluracil and 5-iodouracil nucleosides, protected as their p-toluoyl esters, gave high yields in the presence of (Ph3P)2PdCl2 and CuI in warm Et3N. Several of the deprotected 5-alkynyl-2'-deoxyuridines, including 5-ethynyl-2'-deoxyuridine, had antiviral activity; their 5'-monophosphates inhibited thymidylate synthetase. Controlled hydrogenation of the 5-alkynyl side chain gave (Z)-5-alkenyl- or the saturated 5-alkyl-2'-deoxyuridines. This provides a stereocontrolled route to the known 5-ethyl- and 5-n-hexyl-2'-deoxyuridines as well as (E)-5-(2-bromovinyl)-2'-deoxyuridine. Hydration of the triple bond sometimes gave uracil-5-alkanones.
IT **77875-84-4P 77875-86-6P 77875-87-7P**
77875-88-8P 77875-89-9P 77875-90-2P
77875-93-5P 77875-94-6P 77875-95-7P
77882-22-5P 85267-64-7P 85267-65-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of)
RN 77875-84-4 CAPLUS
CN Uridine, 5-[4-[(4-methylbenzoyl)oxy]-1-butynyl]-, 2',3',5'-tris(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

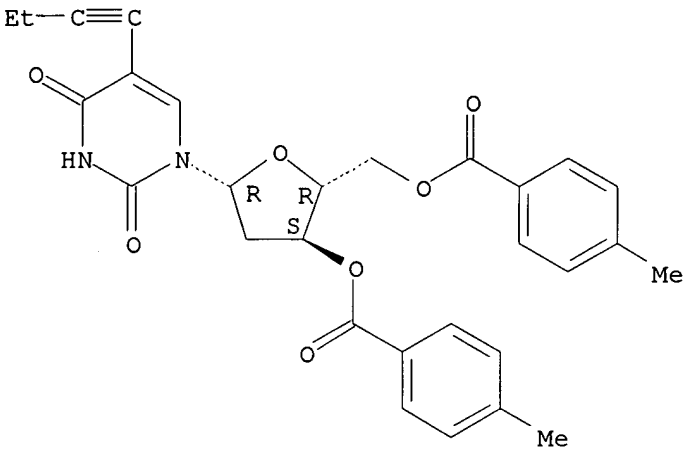
PAGE 1-A





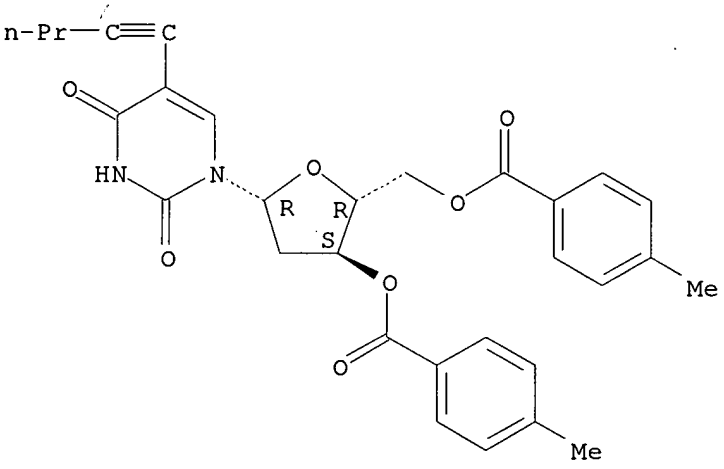
RN 77875-86-6 CAPLUS
CN Uridine, 5-(1-butynyl)-2'-deoxy-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 77875-87-7 CAPLUS
CN Uridine, 2'-deoxy-5-(1-pentynyl)-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

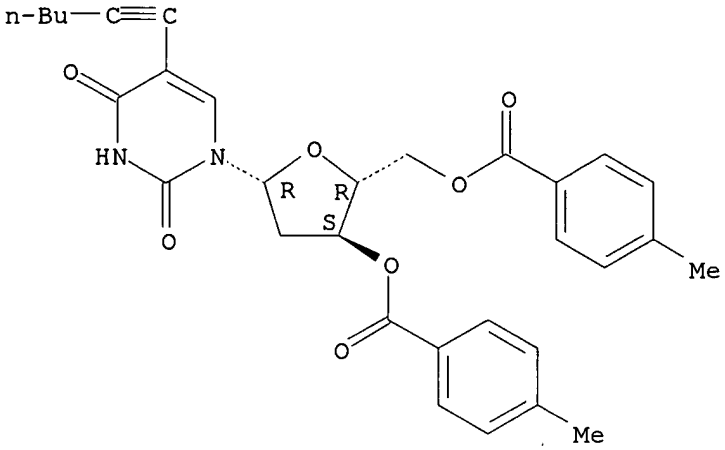
Absolute stereochemistry.



RN 77875-88-8 CAPLUS
CN Uridine, 2'-deoxy-5-(1-hexynyl)-, 3',5'-bis(4-methylbenzoate) (9CI) (CA

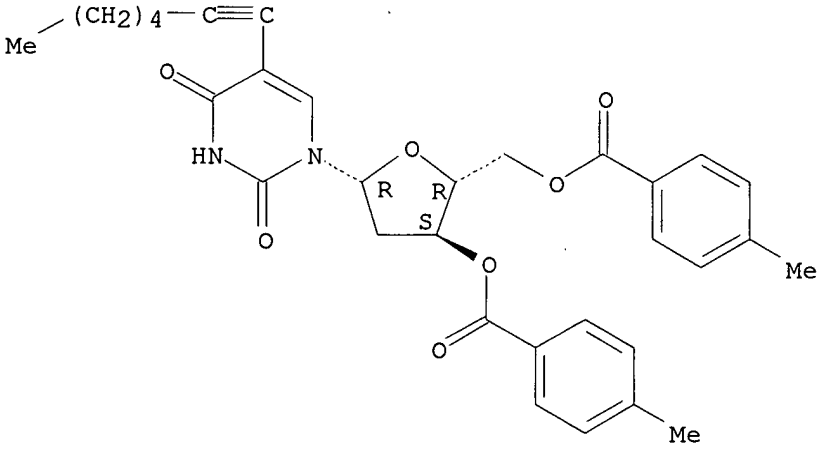
INDEX NAME)

Absolute stereochemistry.



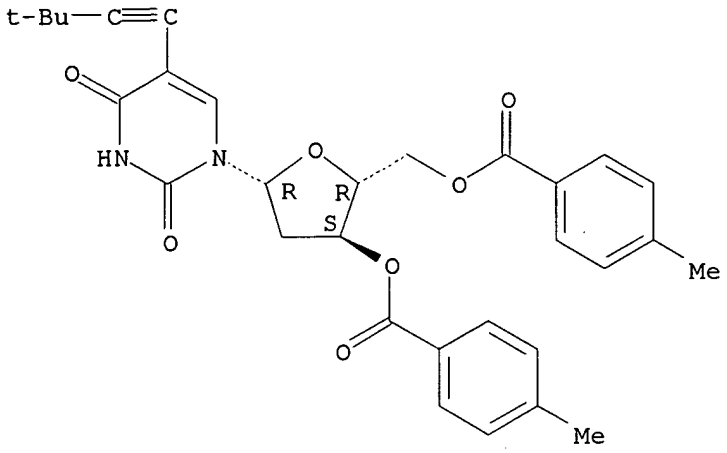
RN 77875-89-9 CAPLUS
CN Uridine, 2'-deoxy-5-(1-heptynyl)-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



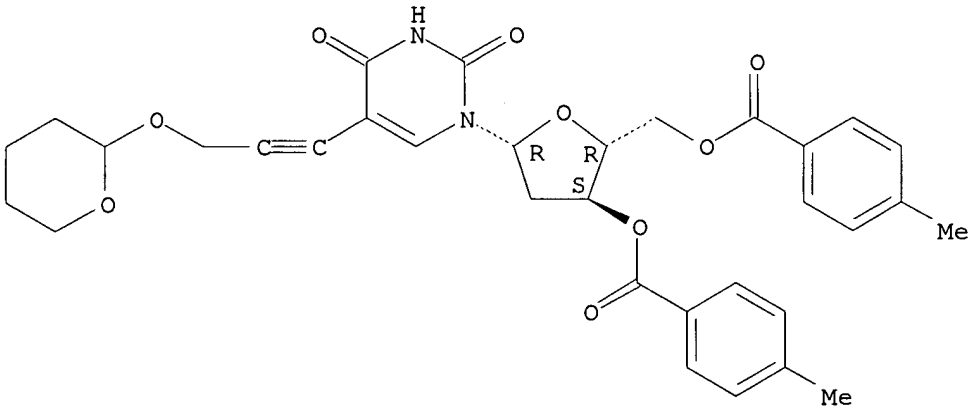
RN 77875-90-2 CAPLUS
CN Uridine, 2'-deoxy-5-(3,3-dimethyl-1-butynyl)-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



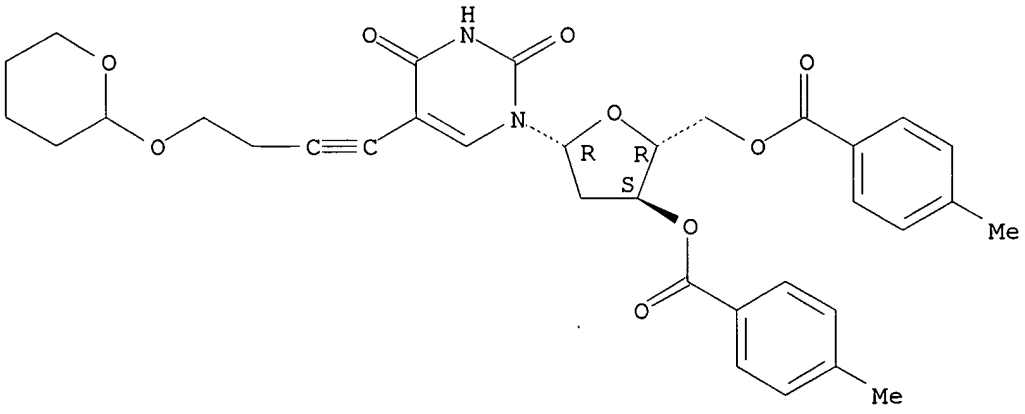
RN 77875-93-5 CAPLUS
CN Uridine, 2'-deoxy-5-[3-[(tetrahydro-2H-pyran-2-yl)oxy]-1-propynyl]-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 77875-94-6 CAPLUS
CN Uridine, 2'-deoxy-5-[4-[(tetrahydro-2H-pyran-2-yl)oxy]-1-butynyl]-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

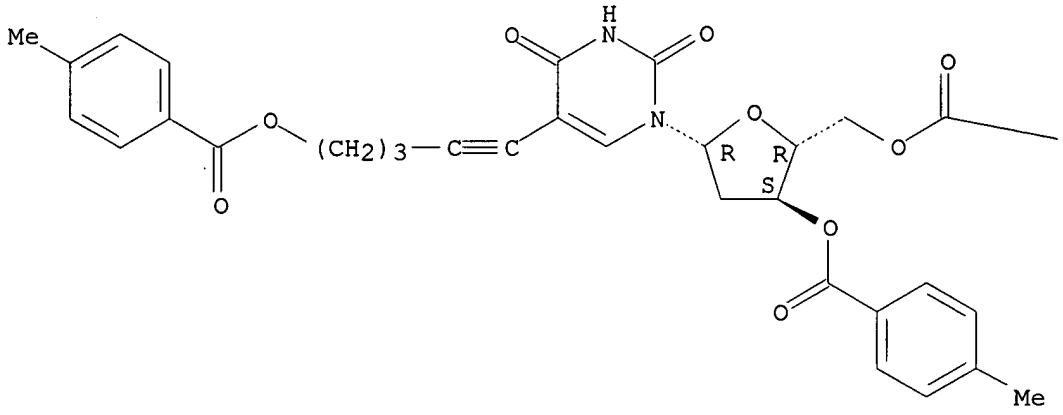
Absolute stereochemistry.



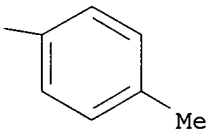
RN 77875-95-7 CAPLUS
CN Uridine, 2'-deoxy-5-[5-[(4-methylbenzoyl)oxy]-1-pentynyl]-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



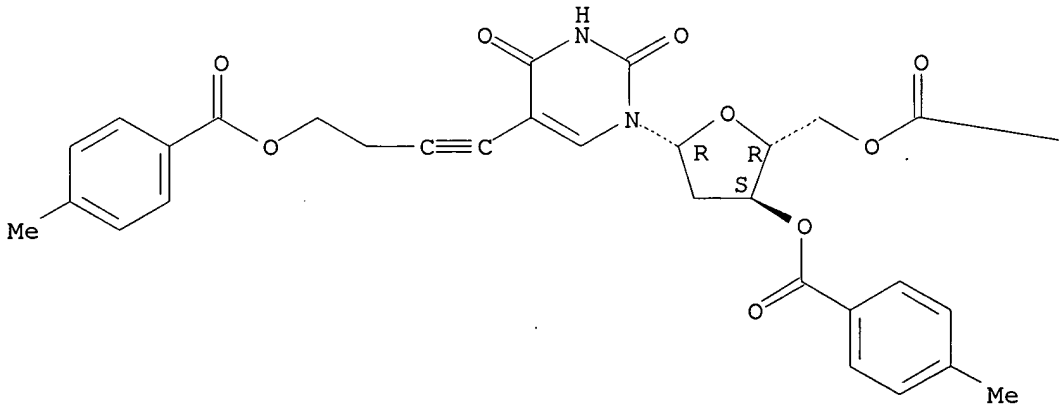
PAGE 1-B

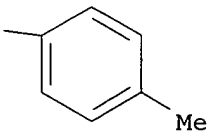


RN 77882-22-5 CAPLUS
CN Uridine, 2'-deoxy-5-[4-[(4-methylbenzoyl)oxy]-1-butynyl]-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

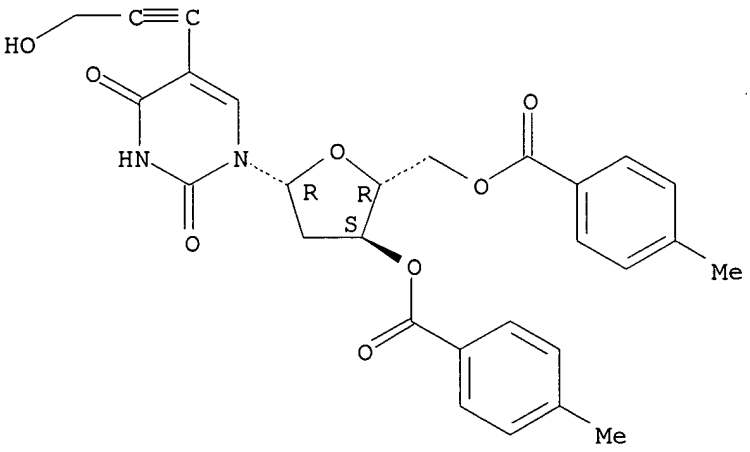
PAGE 1-A





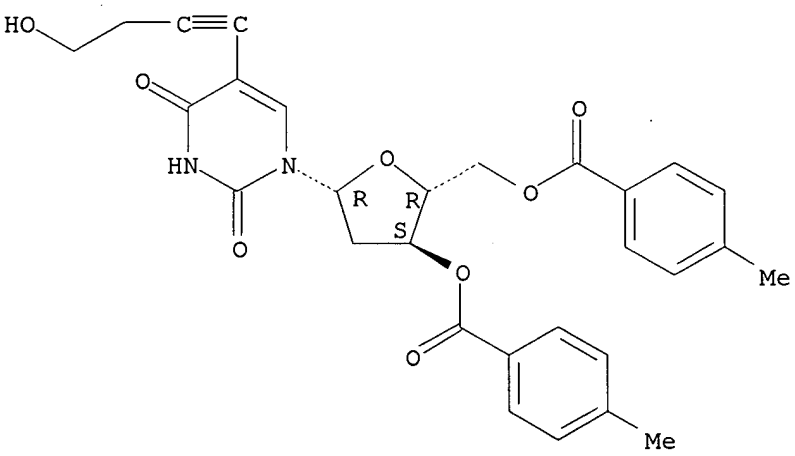
RN 85267-64-7 CAPLUS
CN Uridine, 2'-deoxy-5-(3-hydroxy-1-propynyl)-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



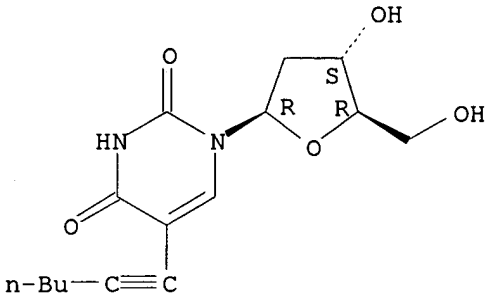
RN 85267-65-8 CAPLUS
CN Uridine, 2'-deoxy-5-(4-hydroxy-1-butynyl)-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



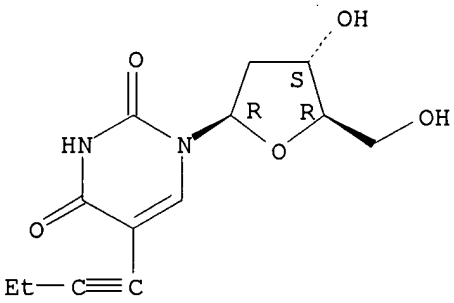
IT **77875-97-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenation of)
RN 77875-97-9 CAPLUS
CN Uridine, 2'-deoxy-5-(1-hexynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



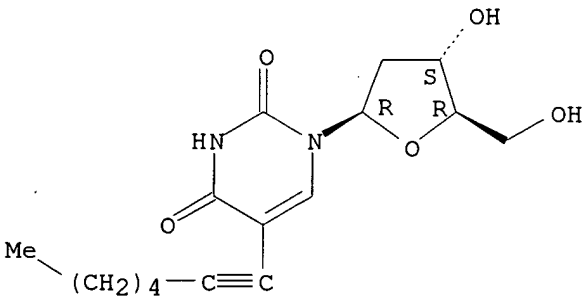
IT **77875-96-8P 77875-98-0P 77875-99-1P**
77876-00-7P 77876-01-8P 77887-18-4P
77887-19-5P 84559-05-7P 84582-78-5P
85267-61-4P 85267-67-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 77875-96-8 CAPLUS
CN Uridine, 5-(1-butynyl)-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 77875-98-0 CAPLUS
CN Uridine, 2'-deoxy-5-(1-heptynyl)- (9CI) (CA INDEX NAME)

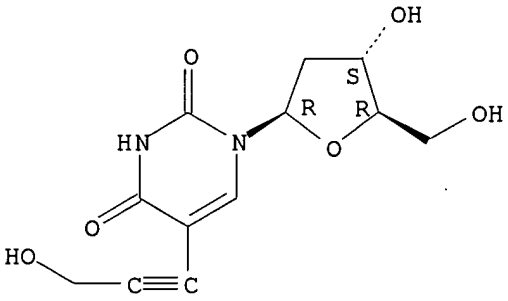
Absolute stereochemistry.



RN 77875-99-1 CAPLUS

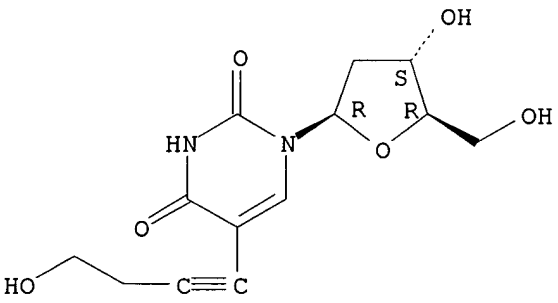
CN Uridine, 2'-deoxy-5-(3-hydroxy-1-propynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



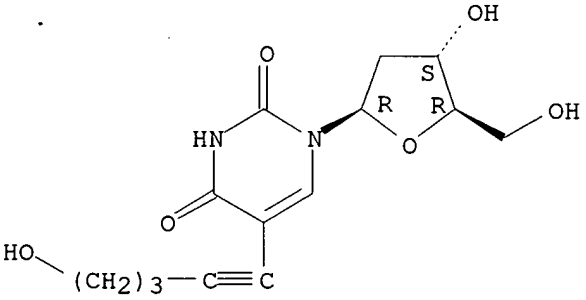
RN 77876-00-7 CAPLUS
CN Uridine, 2'-deoxy-5-(4-hydroxy-1-butynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



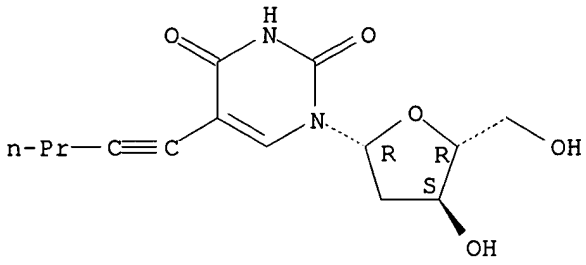
RN 77876-01-8 CAPLUS
CN Uridine, 2'-deoxy-5-(5-hydroxy-1-pentynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



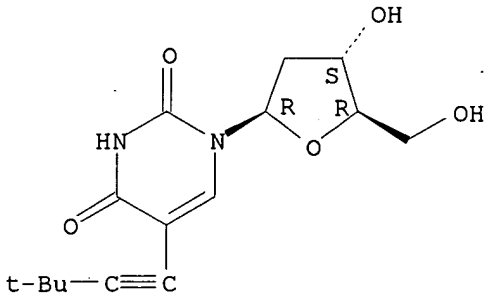
RN 77887-18-4 CAPLUS
CN Uridine, 2'-deoxy-5-(1-pentynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



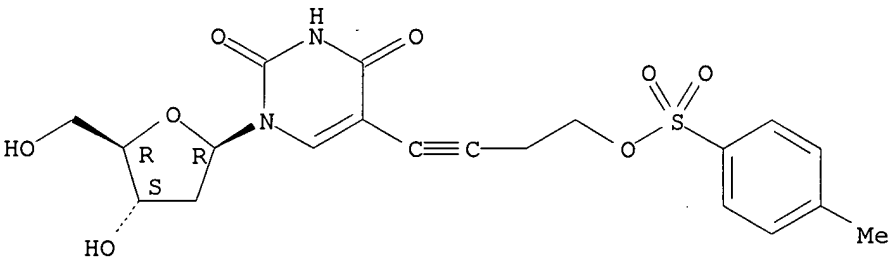
RN 77887-19-5 CAPLUS
CN Uridine, 2'-deoxy-5-(3,3-dimethyl-1-butynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



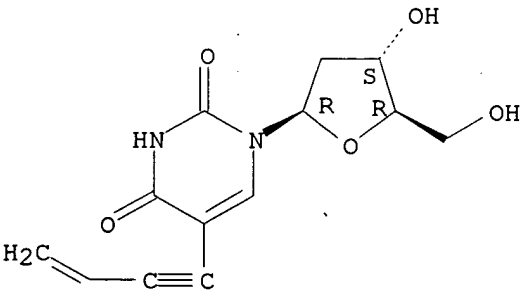
RN 84559-05-7 CAPLUS
CN Uridine, 2'-deoxy-5-[4-[[(4-methylphenyl)sulfonyl]oxy]-1-butynyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



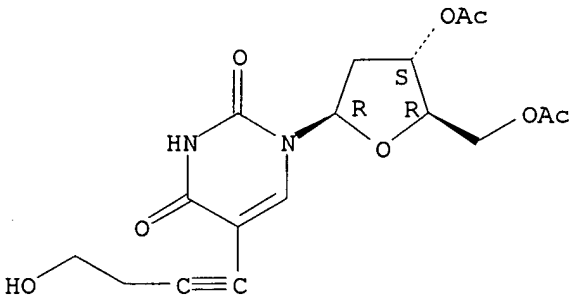
RN 84582-78-5 CAPLUS
CN Uridine, 5-(3-buten-1-ynyl)-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



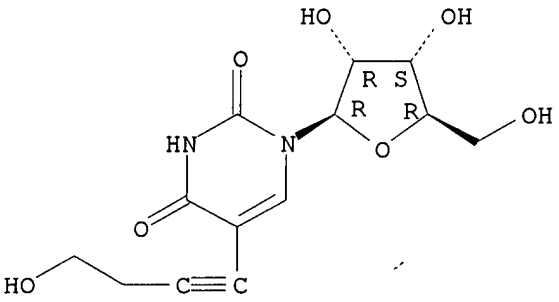
RN 85267-61-4 CAPLUS
CN Uridine, 2'-deoxy-5-(4-hydroxy-1-butynyl)-, 3',5'-diacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 85267-67-0 CAPLUS
CN Uridine, 5-(4-hydroxy-1-butynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

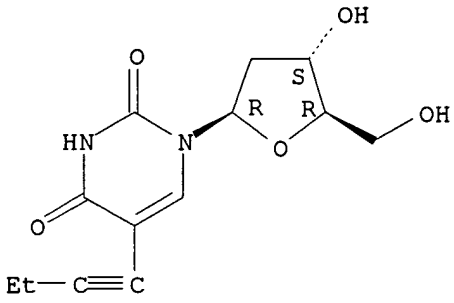


L9 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:198636 CAPLUS
DN 98:198636
TI **Nucleic acid** related compounds. 40. Synthesis and biological activities of 5-alkynyluracil nucleosides
AU De Clercq, Erik; Descamps, Johan; Balzarini, Jan; Giziewicz, Jerzy; Barr, Philip J.; Robins, Morris J.
CS Rega Inst. Med. Res., Kathol. Univ., Louvain, B-3000, Belg.
SO Journal of Medicinal Chemistry (**1983**), 26(5), 661-6
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
AB Coupling of terminal alkynes with 5-iodo-1-(2,3,5-tri-O-p-toluoyl-β-D-arabinofuranosyl)uracil and 5-iodo-3',5'-di-O-p-toluoyl-2'-deoxyuridine proceeded readily in Et3N with catalytic (Ph3P)2PdCl2 and CuI. Deprotection gave 5-alkynyl-1-β-D-arabinofuranosyluracil and 5-alkynyl-2'-deoxyuridine nucleosides. The 5-ethynyl, followed by 5-propynyl, products had the highest antiviral potency, with the 2'-deoxy derivs. being more effective than the arabinosyl compds. Activity was weak at hexynyl and disappeared at heptynyl. Inclusion of an ω-hydroxy function diminished the antiviral effect. None of the 5-alkynyluracil nucleosides tested had sufficient selectivity to qualify as a candidate antiviral drug. Several of the compds. inhibited thymidylate synthetase, with 5-ethynyl-2'-deoxyuridine being the most cytotoxic against L1210 cells.
IT **77875-96-8 77875-97-9 77875-98-0**

77875-99-1 77876-00-7 77876-01-8
77887-18-4 77887-19-5 84559-05-7
84582-78-5
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(antiviral, antimetabolic, and antileukemia activity of)

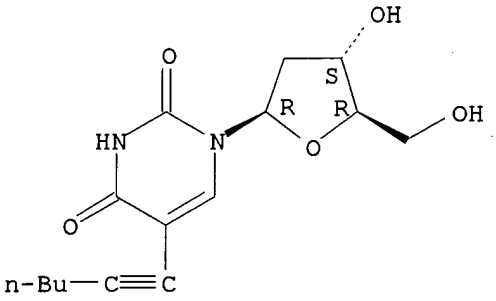
RN 77875-96-8 CAPLUS
CN Uridine, 5-(1-butynyl)-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



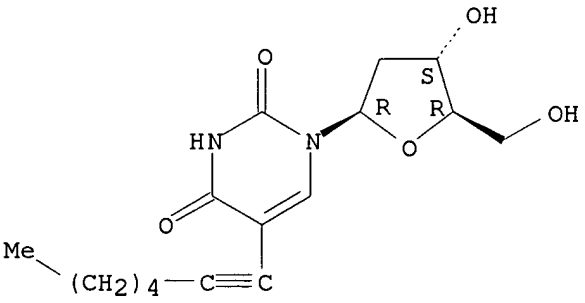
RN 77875-97-9 CAPLUS
CN Uridine, 2'-deoxy-5-(1-hexynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



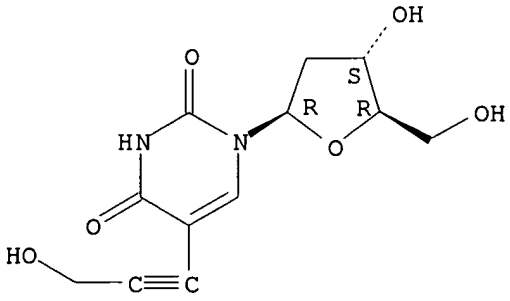
RN 77875-98-0 CAPLUS
CN Uridine, 2'-deoxy-5-(1-heptynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



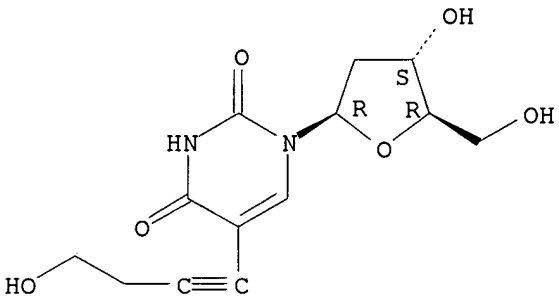
RN 77875-99-1 CAPLUS
CN Uridine, 2'-deoxy-5-(3-hydroxy-1-propynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



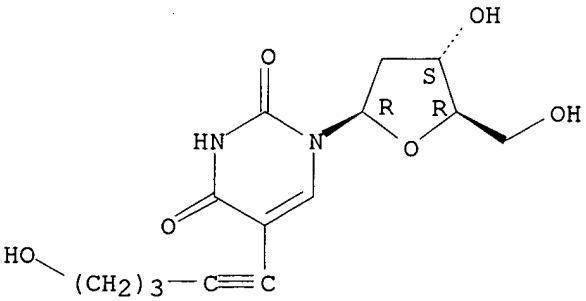
RN 77876-00-7 CAPLUS
CN Uridine, 2'-deoxy-5-(4-hydroxy-1-butynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



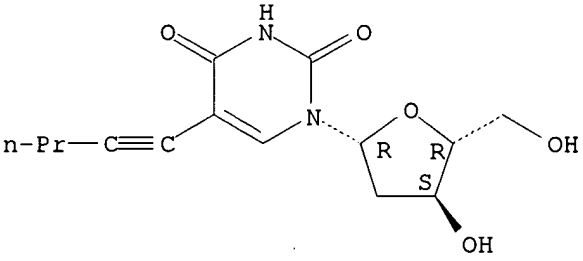
RN 77876-01-8 CAPLUS
CN Uridine, 2'-deoxy-5-(5-hydroxy-1-pentynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



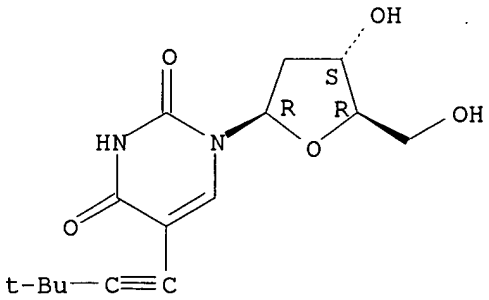
RN 77887-18-4 CAPLUS
CN Uridine, 2'-deoxy-5-(1-pentynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



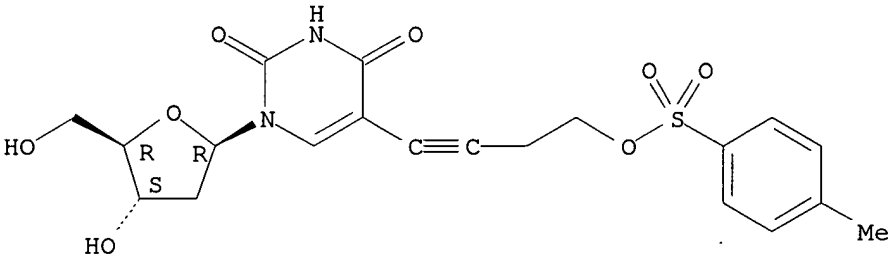
RN 77887-19-5 CAPLUS
CN Uridine, 2'-deoxy-5-(3,3-dimethyl-1-butynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



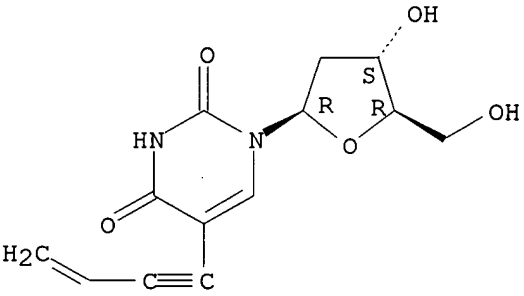
RN 84559-05-7 CAPLUS
CN Uridine, 2'-deoxy-5-[4-[[(4-methylphenyl)sulfonyl]oxy]-1-butynyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



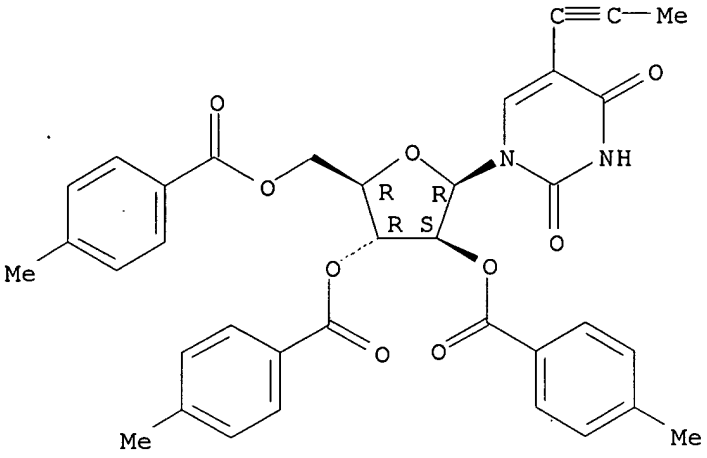
RN 84582-78-5 CAPLUS
CN Uridine, 5-(3-buten-1-ynyl)-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



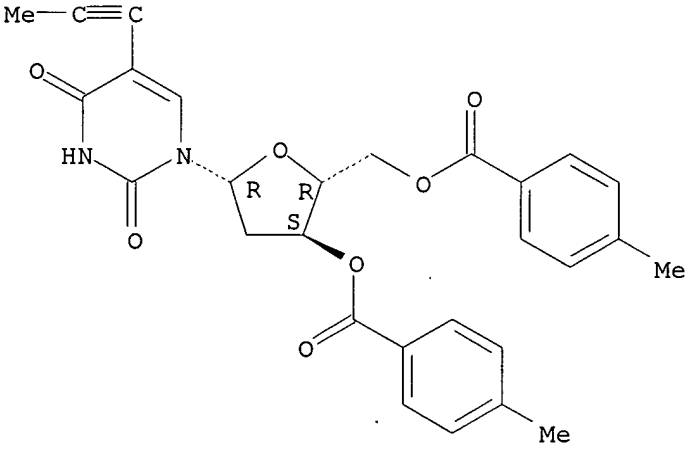
IT **84558-91-8P 84558-92-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of)
RN 84558-91-8 CAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 5-(1-propynyl)-1-[2,3,5-tris-O-(4-methylbenzoyl)-β-D-arabinofuranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



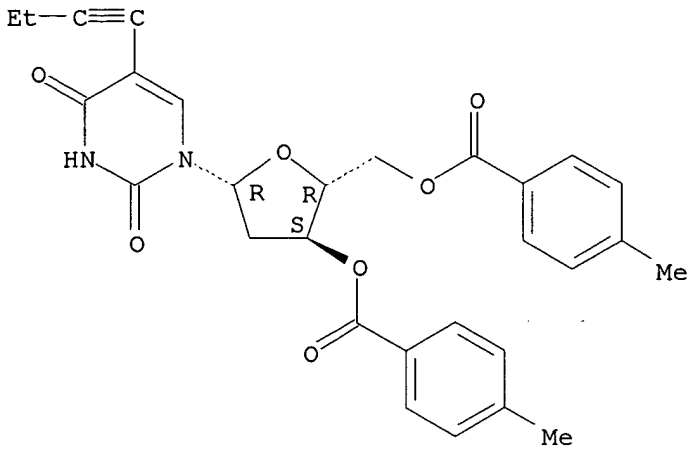
RN 84558-92-9 CAPLUS
CN Uridine, 2'-deoxy-5-(1-propynyl)-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



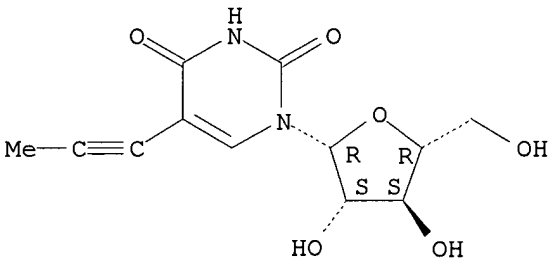
IT **77875-86-6P 84558-93-0P 84558-95-2P**
84558-96-3P 84558-97-4P 84558-98-5P
84558-99-6P 84559-00-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 77875-86-6 CAPLUS
CN Uridine, 5-(1-butynyl)-2'-deoxy-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



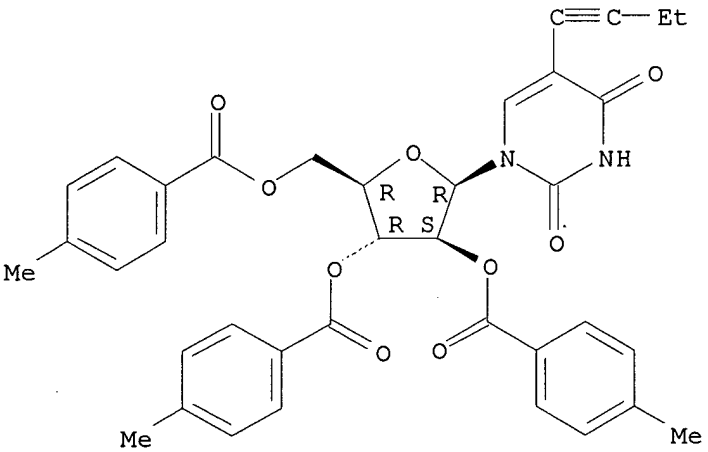
RN 84558-93-0 CAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 1-β-D-arabinofuranosyl-5-(1-propynyl)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



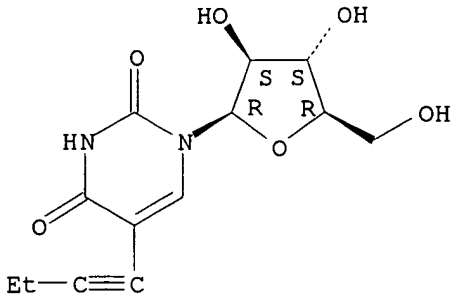
RN 84558-95-2 CAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 5-(1-butynyl)-1-[2,3,5-tris-O-(4-
methylbenzoyl)-β-D-arabinofuranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



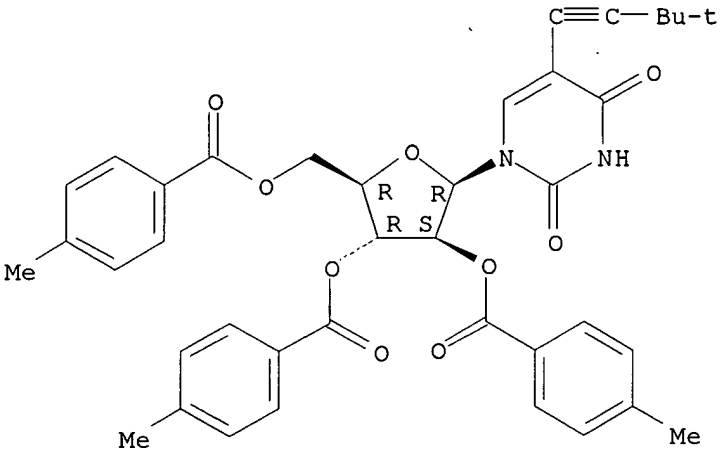
RN 84558-96-3 CAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 1-β-D-arabinofuranosyl-5-(1-butynyl)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



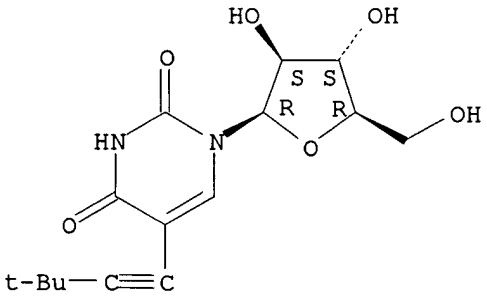
RN 84558-97-4 CAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 5-(3,3-dimethyl-1-butynyl)-1-[2,3,5-tris-O-(4-methylbenzoyl)-β-D-arabinofuranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



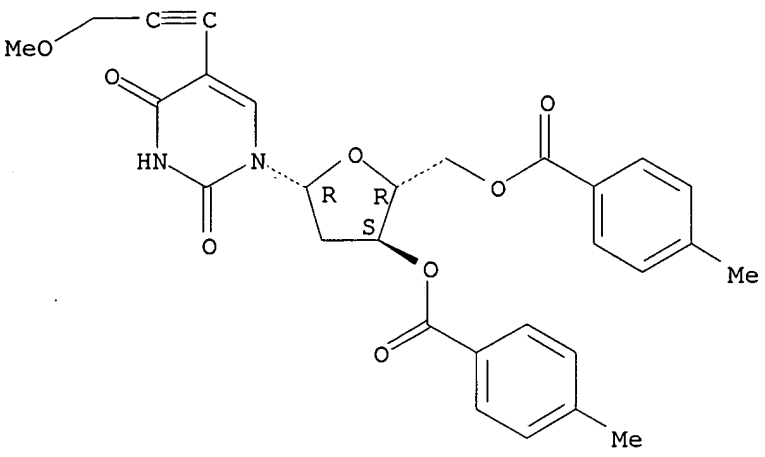
RN 84558-98-5 CAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 1-β-D-arabinofuranosyl-5-(3,3-dimethyl-1-butynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



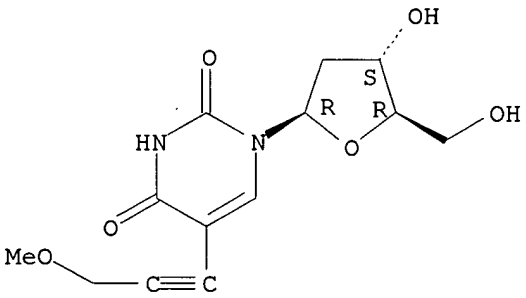
RN 84558-99-6 CAPLUS
CN Uridine, 2'-deoxy-5-(3-methoxy-1-propynyl)-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



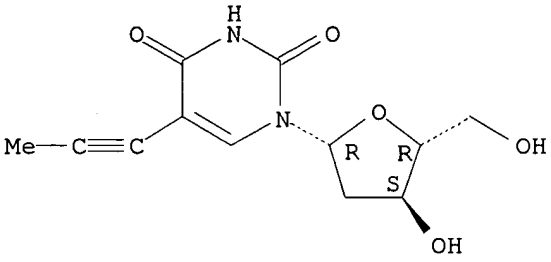
RN 84559-00-2 CAPLUS
CN Uridine, 2'-deoxy-5-(3-methoxy-1-propynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **84558-94-1**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(prepn.and antiviral, antimetabolic, and antileukemia activity of)
RN 84558-94-1 CAPLUS
CN Uridine, 2'-deoxy-5-(1-propynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



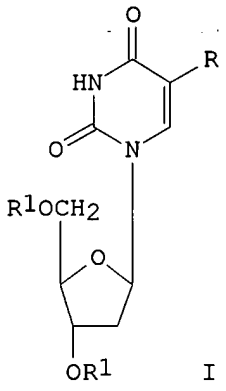
L9 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1981:407669 CAPLUS
DN 95:7669
TI **Nucleic acid** related compounds. 31. Smooth and efficient palladium-copper catalyzed coupling of terminal alkynes with

5-iodouracil nucleosides

AU Robins, Morris J.; Barr, Philip J.
CS Dep. Chem., Univ. Alberta, Edmonton, AB, T6G 2G2, Can.

SO Tetrahedron Letters (**1981**), 22(5), 421-4
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English

GI



I

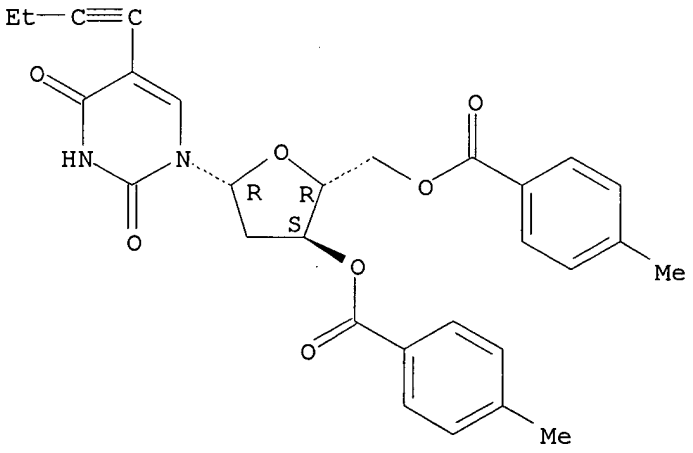
AB Reaction of terminal alkynes with protected uridines in the presence of Pd and Cu gave the corresponding 5-(alkyn-1-yl)uracil nucleosides in 72-92% yield. E.g., uridine I (R = iodo, R1 = p-MeC6H4) coupled with EtC.tplbond.CH in Et3N at 50° under N for 10 h in the presence of (Ph3P)PdCl2 and CuI to give 91% I (R = C.tplbond.CEt, R1 = p-MeC6H4) which was deprotected to give I (R = C.tplbond.CEt, R1 = H).

IT **77875-86-6P 77875-87-7P 77875-88-8P**
77875-89-9P 77875-90-2P 77875-93-5P
77875-94-6P 77875-95-7P 77882-22-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of)

RN 77875-86-6 CAPLUS

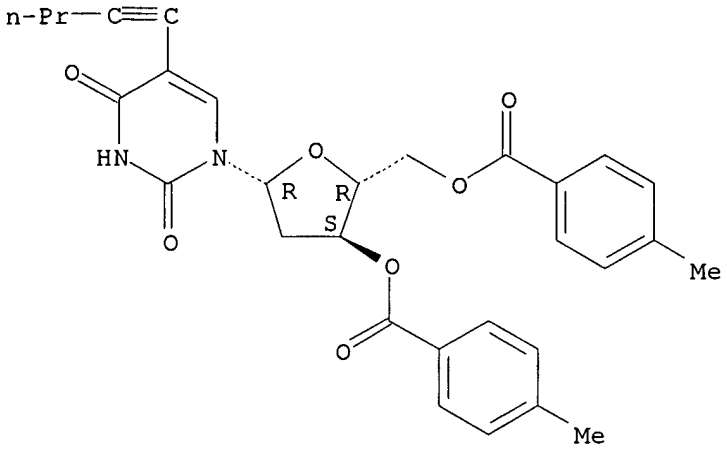
CN Uridine, 5-(1-butynyl)-2'-deoxy-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



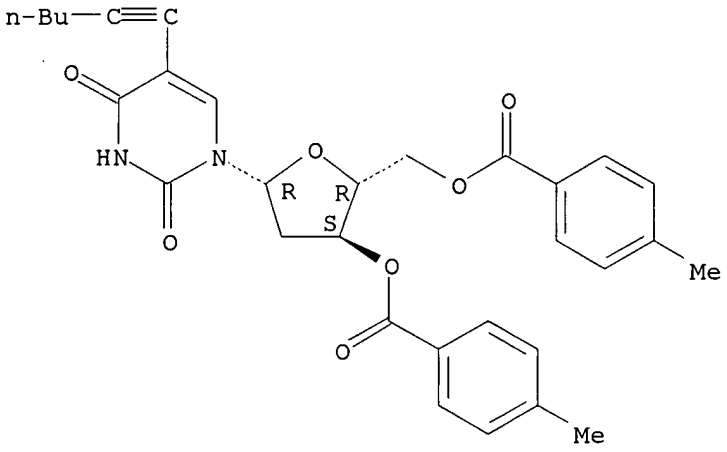
RN 77875-87-7 CAPLUS
CN Uridine, 2'-deoxy-5-(1-pentynyl)-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



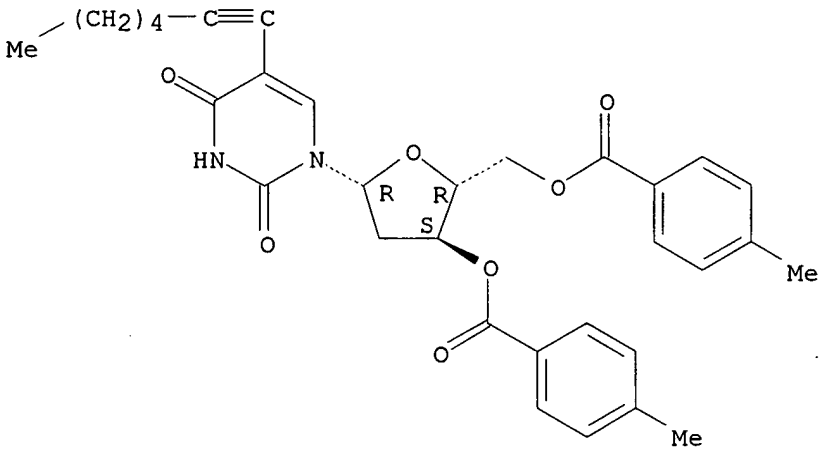
RN 77875-88-8 CAPLUS
CN Uridine, 2'-deoxy-5-(1-hexynyl)-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



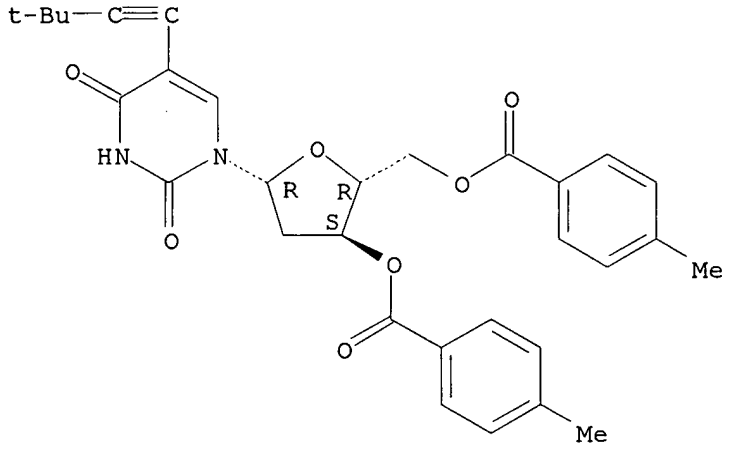
RN 77875-89-9 CAPLUS
CN Uridine, 2'-deoxy-5-(1-heptynyl)-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



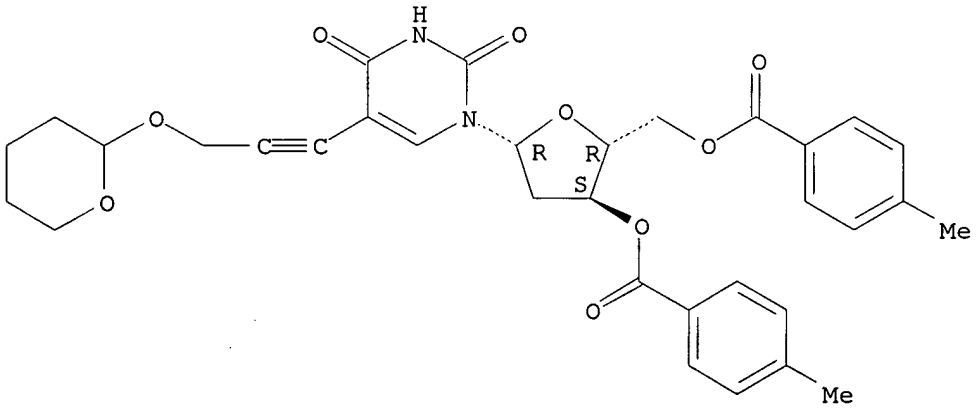
RN 77875-90-2 CAPLUS
CN Uridine, 2'-deoxy-5-(3,3-dimethyl-1-butynyl)-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



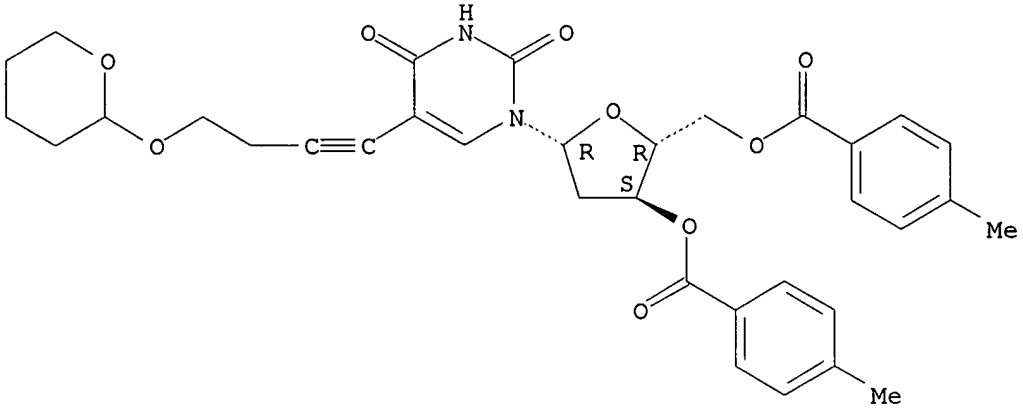
RN 77875-93-5 CAPLUS
CN Uridine, 2'-deoxy-5-[3-[(tetrahydro-2H-pyran-2-yl)oxy]-1-propynyl]-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 77875-94-6 CAPLUS
CN Uridine, 2'-deoxy-5-[4-[(tetrahydro-2H-pyran-2-yl)oxy]-1-butynyl]-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

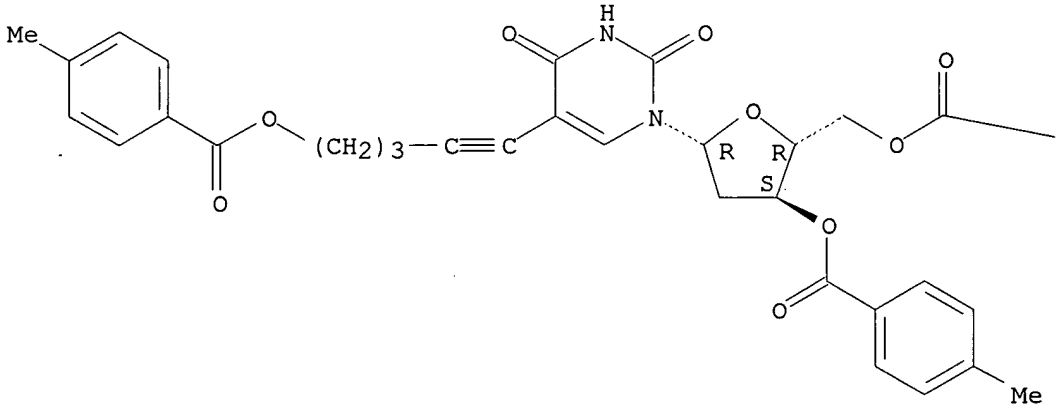
Absolute stereochemistry.



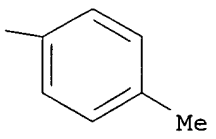
RN 77875-95-7 CAPLUS
CN Uridine, 2'-deoxy-5-[5-[(4-methylbenzoyl)oxy]-1-pentynyl]-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

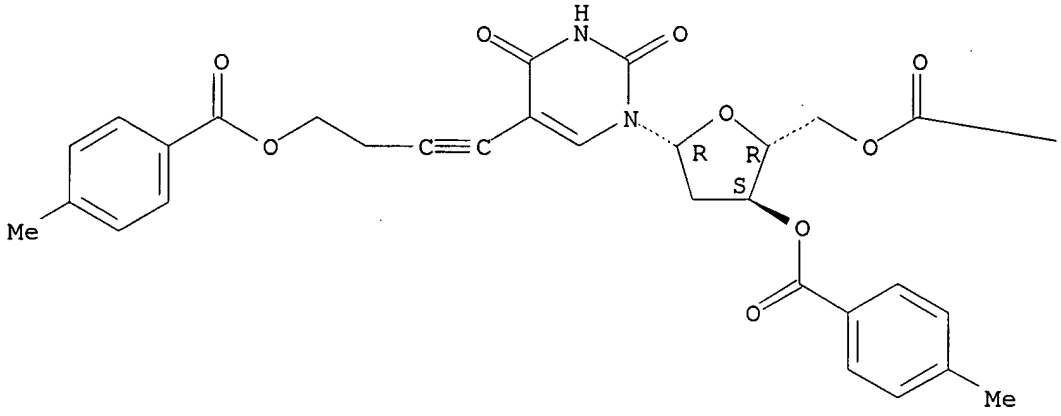


RN 77882-22-5 CAPLUS

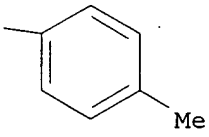
CN Uridine, 2'-deoxy-5-[4-[(4-methylbenzoyl)oxy]-1-butynyl]-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



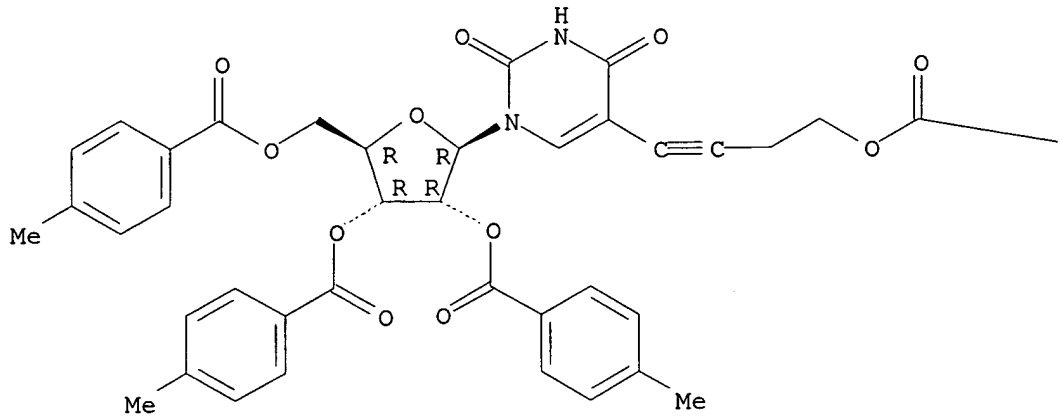
PAGE 1-B



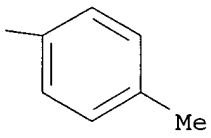
IT **77875-84-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by alkynylation of uridine)
RN 77875-84-4 CAPLUS
CN Uridine, 5-[4-[(4-methylbenzoyl)oxy]-1-butynyl]-, 2',3',5'-tris(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

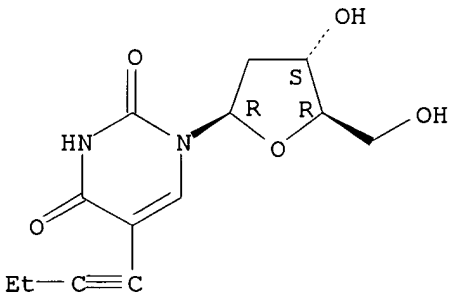


PAGE 1-B



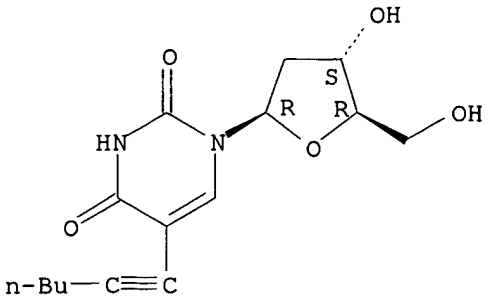
IT **77875-96-8P 77875-97-9P 77875-98-0P**
77875-99-1P 77876-00-7P 77876-01-8P
77887-18-4P 77887-19-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by alkynylation/deprotection of iodouridine)
RN 77875-96-8 CAPLUS
CN Uridine, 5-(1-butynyl)-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



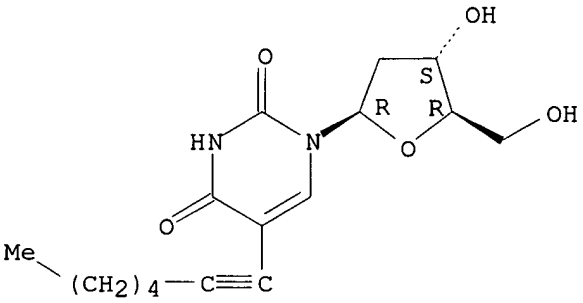
RN 77875-97-9 CAPLUS
CN Uridine, 2'-deoxy-5-(1-hexynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



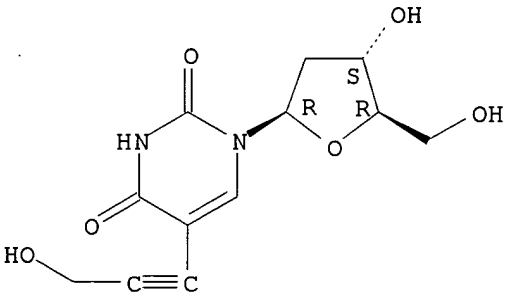
RN 77875-98-0 CAPLUS
CN Uridine, 2'-deoxy-5-(1-heptynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



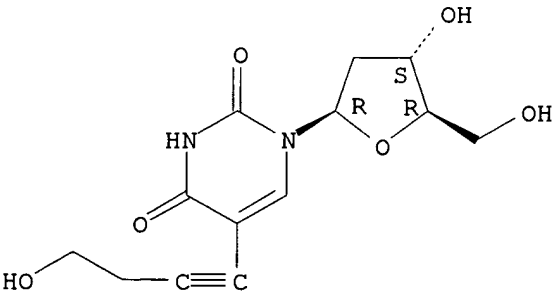
RN 77875-99-1 CAPLUS
CN Uridine, 2'-deoxy-5-(3-hydroxy-1-propynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



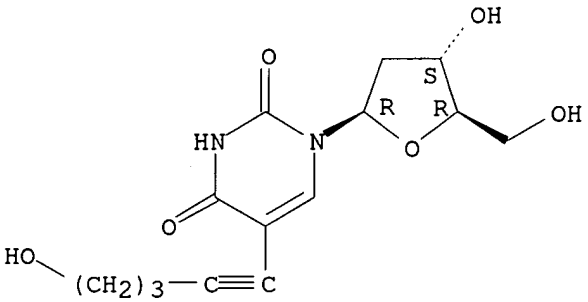
RN 77876-00-7 CAPLUS
CN Uridine, 2'-deoxy-5-(4-hydroxy-1-butynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



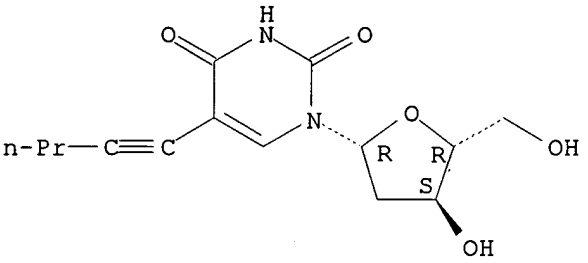
RN 77876-01-8 CAPLUS
CN Uridine, 2'-deoxy-5-(5-hydroxy-1-pentynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



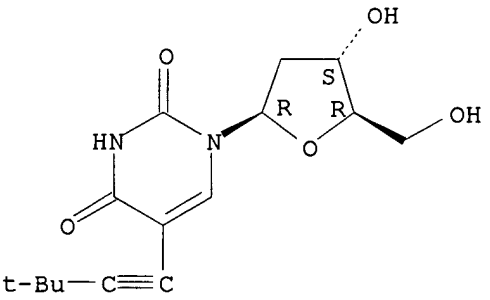
RN 77887-18-4 CAPLUS
CN Uridine, 2'-deoxy-5-(1-pentynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 77887-19-5 CAPLUS
CN Uridine, 2'-deoxy-5-(3,3-dimethyl-1-butynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d his

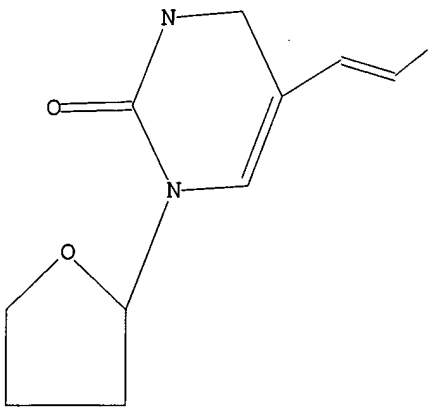
(FILE 'HOME' ENTERED AT 09:00:10 ON 28 DEC 2004)

FILE 'REGISTRY' ENTERED AT 09:00:17 ON 28 DEC 2004
L1 STRUCTURE UPLOADED
L2 1171 S L1 FULL

FILE 'CAPLUS' ENTERED AT 09:00:43 ON 28 DEC 2004
L3 415 S L2

```
L4          123 S L3 AND NUCLEIC ACID
L5          123 DUP REM L4 (0 DUPLICATES REMOVED)
L6          123 S L5
L7            5 S L5 AND PY=1993
L8          123 S L5
L9           15 S L5 AND PY<=1993

=>
```

```
=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                   750.24     905.87

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY    SESSION
CA SUBSCRIBER PRICE                                  -109.90    -109.90

FILE 'REGISTRY' ENTERED AT 09:35:34 ON 28 DEC 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   26 DEC 2004  HIGHEST RN 802853-20-9
DICTIONARY FILE UPDATES:  26 DEC 2004  HIGHEST RN 802853-20-9

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

*** YOU HAVE NEW MAIL ***

=>
Uploading C:\Program Files\Stnexp\Queries\107306431.str

L10     STRUCTURE UPLOADED

=> d l10
L10 HAS NO ANSWERS
L10             STR
```



Structure attributes must be viewed using STN Express query preparation.

```
=> s l10 full
FULL SEARCH INITIATED 09:36:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   1312 TO ITERATE

100.0% PROCESSED    1312 ITERATIONS                          967 ANSWERS
SEARCH TIME: 00.00.01

L11          967 SEA SSS FUL L10

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               155.84    1061.71

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
                                                   ENTRY    SESSION
CA SUBSCRIBER PRICE                                0.00    -109.90

FILE 'CAPLUS' ENTERED AT 09:36:31 ON 28 DEC 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)
```



```
FILE COVERS 1907 - 28 Dec 2004  VOL 142 ISS 1
FILE LAST UPDATED: 24 Dec 2004  (20041224/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s l11
L12          703 L11

=> dup rem l12
PROCESSING COMPLETED FOR L12
L13           702 DUP REM L12 (1 DUPLICATE REMOVED)

=> s l13 and nucleic acid
L14          702 S L13
          163616 NUCLEIC
         3916487 ACID
          117879 NUCLEIC ACID
                 (NUCLEIC(W)ACID)
L15          320 L14 AND NUCLEIC ACID

=> s l15 and py<=1993
       15254580 PY<=1993
L16          107 L15 AND PY<=1993
```

FILE 'HOME' ENTERED AT 09:55:13 ON 28 DEC 2004

=> file reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 09:55:21 ON 28 DEC 2004

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 26 DEC 2004 HIGHEST RN 802853-20-9
DICTIONARY FILE UPDATES: 26 DEC 2004 HIGHEST RN 802853-20-9

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

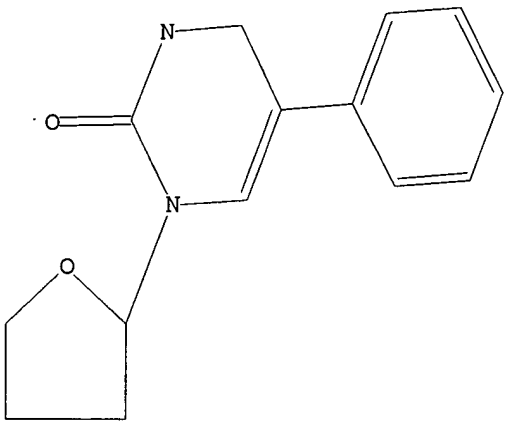
Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

*** YOU HAVE NEW MAIL ***

=>
Uploading C:\Program Files\Stnexp\Queries\107306432.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

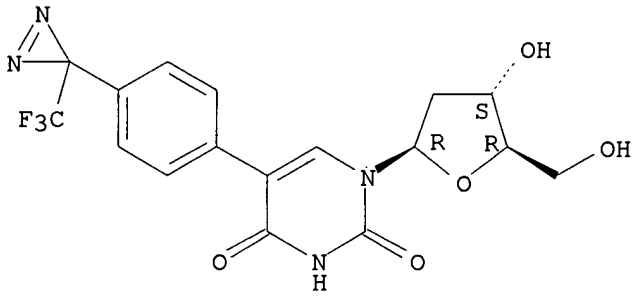
```
=> s l1 full
FULL SEARCH INITIATED 09:55:43 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   1372 TO ITERATE

100.0% PROCESSED    1372 ITERATIONS                          234 ANSWERS
SEARCH TIME: 00.00.01

L2          234 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               155.42     155.63

FILE 'CAPLUS' ENTERED AT 09:55:54 ON 28 DEC 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)
```



```
FILE COVERS 1907 - 28 Dec 2004  VOL 142 ISS 1
FILE LAST UPDATED: 24 Dec 2004  (20041224/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s l2
L3          71 L2

=> dup rem l3
PROCESSING COMPLETED FOR L3
L4           70 DUP REM L3 (1 DUPLICATE REMOVED)

=> s l4 and nucleic acid
L5          70 S L4
        163616 NUCLEIC
       3916487 ACID
        117879 NUCLEIC ACID
                 (NUCLEIC(W)ACID)
L6          12 L5 AND NUCLEIC ACID

=> d l6 bib abs hitstr 1-12

L6   ANSWER 1 OF 12  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   2003:584281  CAPLUS
DN   139:257146
TI   Photochemical cross-linking of Escherichia coli Fpg protein to DNA
     duplexes containing phenyl(trifluoromethyl)diazirine groups
AU   Taranenko, Maria; Rykhlevskaya, Anna; Mtchedlidze, Manana; Laval, Jacques;
     Kuznetsova, Svetlana
CS   Laboratory of Nucleic Acids Chemistry, Department of Chemistry, Moscow
```

State University, Moscow, Russia
SO European Journal of Biochemistry (2003), 270(14), 2945-2949
CODEN: EJBCAI; ISSN: 0014-2956
PB Blackwell Publishing Ltd.
DT Journal
LA English
AB Formamidopyrimidine-DNA glycosylase (Fpg protein) of Escherichia coli is a DNA repair enzyme that excises oxidized purine bases, most notably the mutagenic 7-hydro-8-oxoguanine, from damaged DNA. In order to identify specific contacts between nucleobases of DNA and amino acids from the E. coli Fpg protein, photochem. crosslinking was employed using new reactive DNA duplexes containing 5-[4-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenyl]-2'-deoxyuridine dU* residues near the 7-hydro-8-oxoguanosine (oxoG) lesion. The Fpg protein was found to bind specifically and tightly to the modified DNA duplexes and to incise them. The nicking efficiency of the DNA duplex containing a dU* residue 5' to the oxoG was higher as compared to oxidized native DNA. The conditions for the photochem. crosslinking of the reactive DNA duplexes and the Fpg protein have been optimized to yield as high as 10% of the cross-linked product. Our results suggest that the Fpg protein forms contacts with two nucleosides, one 5' adjacent to oxoG and the other 5' adjacent to the cytidine residue pairing with oxoG in the other strand. The approaches developed may be applicable to pro- and eukaryotic homologs of the E. coli Fpg protein as well as to other repair enzymes.
IT **210107-39-4**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(Escherichia coli formamidopyrimidine-DNA glycosylase forms contacts with two nucleosides, one 5' adjacent to oxoG and other 5' adjacent to cytidine residue pairing with oxoG in other strand)
RN 210107-39-4 CAPLUS
CN Uridine, 2'-deoxy-5-[4-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

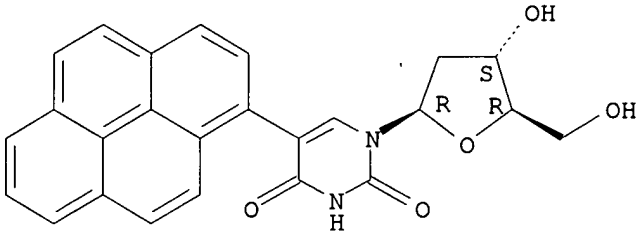


RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:534251 CAPLUS
DN 140:249471
TI Pyrene as a fluorescent probe for DNA base radicals
AU Huber, Robert; Fiebig, Torsten; Wagenknecht, Hans-Achim
CS Institute for Organic Chemistry and Biochemistry, Technical University of Munich, Garching, D-85747, Germany
SO Chemical Communications (Cambridge, United Kingdom) (2003), (15), 1878-1879
CODEN: CHCOFS; ISSN: 1359-7345
PB Royal Society of Chemistry
DT Journal

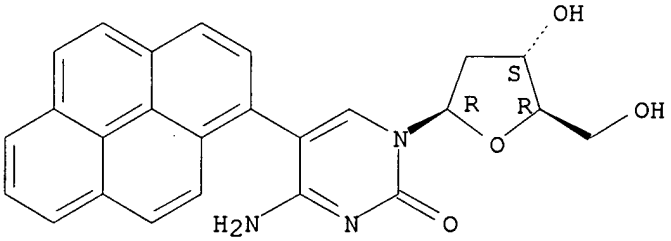
LA English
AB The steady-state emission spectra of 5-(1-pyrenyl)-modified pyrimidine and 8-(1-pyrenyl)-modified purine nucleosides in water at different pH values provide important information about the acidity or basicity of photochem. generated DNA base radicals which are key intermediates in DNA-mediated charge transport processes.
IT **167105-67-1 654668-75-4**
RL: BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); BIOL (Biological study); PROC (Process)
(pyrene as a fluorescent probe for DNA base radicals)
RN 167105-67-1 CAPLUS
CN Uridine, 2'-deoxy-5-(1-pyrenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 654668-75-4 CAPLUS
CN Cytidine, 2'-deoxy-5-(1-pyrenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:876122 CAPLUS
DN 138:182628
TI Electron injection into DNA: Synthesis and spectroscopic properties of pyrenyl-modified oligonucleotides
AU Amann, Nicole; Pandurski, Evgeni; Fiebig, Torsten; Wagenknecht, Hans-Achim
CS Institute for Organic Chemistry and Biochemistry, Technical University of Munich, Garching, 85747, Germany
SO Chemistry--A European Journal (2002), 8(21), 4877-4883
CODEN: CEUJED; ISSN: 0947-6539
PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA English
OS CASREACT 138:182628
AB The nucleoside 5-(1-pyrenyl)-2'-deoxyuridine (1) was prepared by a Suzuki - Miyaura cross-coupling reaction and subsequently used as a DNA building block in order to prepare a range of modified oligonucleotides using

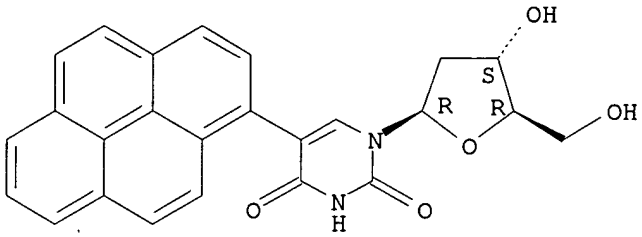
phosphoramidite chemical The DNA duplexes contain a pyrenyl group covalently attached to the nucleobase uracil. Upon excitation at 340 nm an intramol. electron transfer from the pyrenyl group to the uracil moiety takes place which represents an injection of an excess electron into the DNA base stack. Based on the results obtained by steady-state fluorescence and time-resolved pump-probe laser spectroscopy it was possible to show that base-to-base electron transfer can occur from the Py-dU group only to adjacent thymines.

IT **167105-67-1P**
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(base-to base electron transfer in DNA using 5-(1-pyrenyl)-2'-deoxyuridine as building block, transfer from pyrenyl-dU group to adjacent thymines)

RN 167105-67-1 CAPLUS

CN Uridine, 2'-deoxy-5-(1-pyrenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

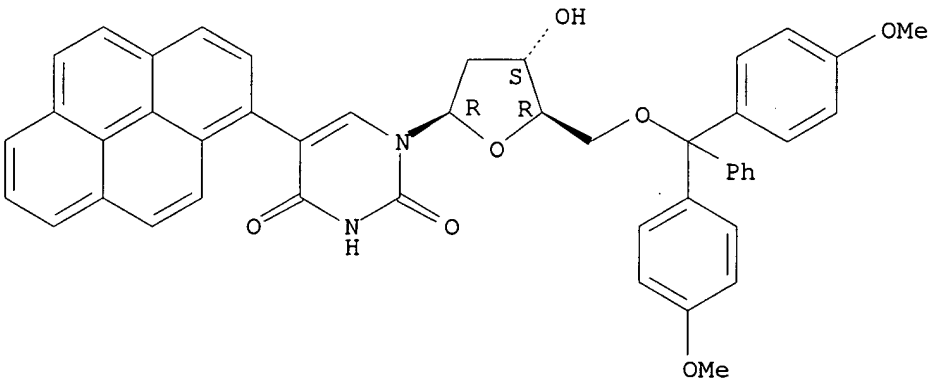


IT **499120-15-9P 499120-16-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(base-to base electron transfer in DNA using 5-(1-pyrenyl)-2'-deoxyuridine as building block, transfer from pyrenyl-dU group to adjacent thymines)

RN 499120-15-9 CAPLUS

CN Uridine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-5-(1-pyrenyl)- (9CI) (CA INDEX NAME)

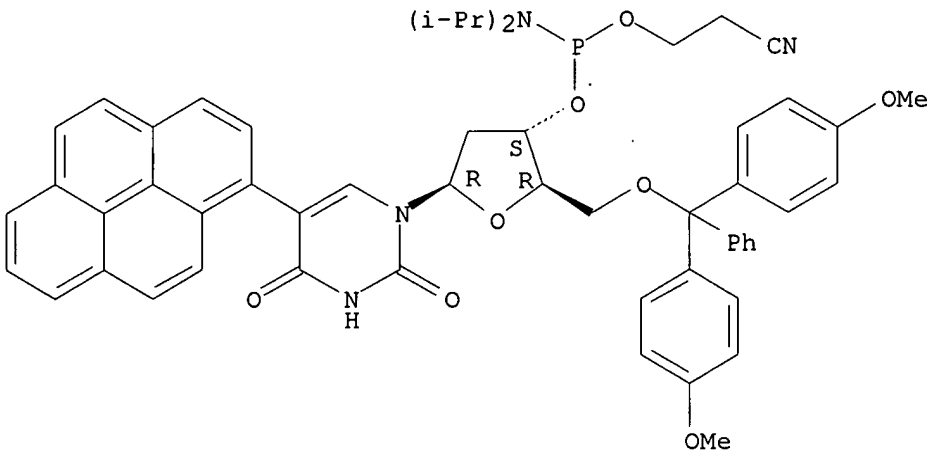
Absolute stereochemistry.



RN 499120-16-0 CAPLUS

CN Uridine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-5-(1-pyrenyl)-, 3'-[2-cyanoethyl bis(1-methylethyl)phosphoramidite] (9CI) (CA INDEX NAME)

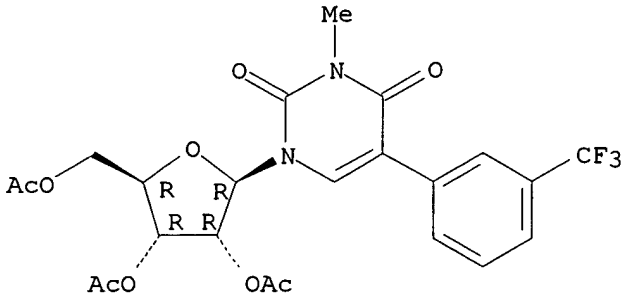
Absolute stereochemistry.



RE.CNT 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:370662 CAPLUS
DN 127:95255
TI Preparation and reactions of new zincated nitrogen-containing heterocycles
AU Prasad, A. S. Bhanu; Stevenson, Thomas M.; Citineni, Janakiram Rao; Nyzam, Valerie; Knochel, Paul
CS Fachbereich Chemie der Philipps, Universitat Marburg, Marburg, 35032, Germany
SO Tetrahedron (1997), 53(21), 7237-7254
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier
DT Journal
LA English
OS CASREACT 127:95255
AB A range of nitrogen-containing iodinated or in some cases brominated heterocycles were converted to the corresponding zincated heterocyclic derivs. by the direct insertion of zinc dust under mild conditions (25°C to 70 °C, 1-3 h) in a solvent like THF or DMAC. This reaction was extended to the preparation of zincated **nucleic acid** bases and nucleosides. The reaction of these new zinc reagents toward various electrophiles with palladium (0) or copper(I) catalysis allows the preparation of a broad range of polyfunctional nitrogen-containing heterocycles.
IT **185386-81-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and catalytic electrophilic addition reactions of zincated nitrogen heterocycles)
RN 185386-81-6 CAPLUS
CN Uridine, 3-methyl-5-[3-(trifluoromethyl)phenyl]-, 2',3',5'-triacetate (9CI) (CA INDEX NAME)

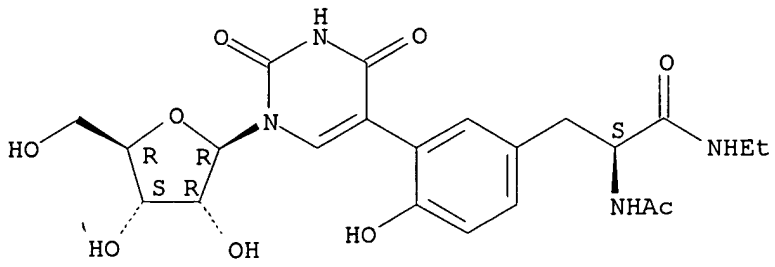
Absolute stereochemistry.



RE.CNT 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

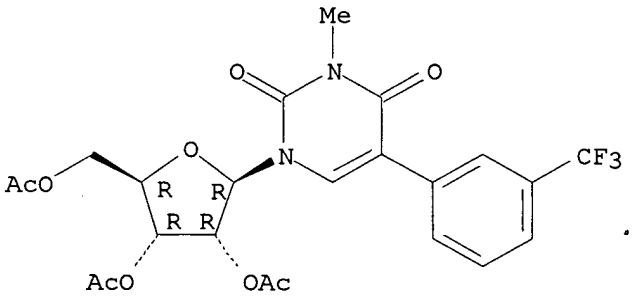
L6 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:143042 CAPLUS
DN 126:260905
TI Mechanistic studies relevant to bromouridine-enhanced nucleoprotein photocrosslinking: possible involvement of an excited tyrosine residue of the protein
AU Norris, Christopher L.; Meisenheimer, Kristen M.; Koch, Tad H.
CS Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO, 80309-0215, USA
SO Photochemistry and Photobiology (1997), 65(2), 201-207
CODEN: PHCBAP; ISSN: 0031-8655
PB American Society for Photobiology
DT Journal
LA English
AB The results of mechanistic studies on formation of uridine (U) and N-acetyl-m-(5-uridinyl)tyrosine N-ethylamide (I) from irradiation of aqueous, pH 7
solns. of bromouridine (BrU) and N-acetyltyrosine N-ethylamide (II) are reported. Solns. were irradiated with monochromatic laser emission at 266, 308, and 325 nm. Quantum yield measurements as a function of excitation wavelength suggest that both products result from excitation of the tyrosine derivative followed by electron transfer to BrU, possibly with intermediacy of the hydrated electron. The BrU radical anion ejects bromide to form the uridinyl radical, which then abstrs. a hydrogen atom from II or adds to the aromatic ring of II. Formation of adduct I is a model for photocrosslinking of nucleic acids bearing the bromouracil chromophore to adjacent tyrosine residues of proteins in nucleoprotein complexes. The value of 325 nm excitation in photocrosslinking, where the tyrosine chromophore is more competitive for photons, was demonstrated with an RNA bound to the MS2 bacteriophage coat protein; >60% increase in the yield of photocrosslinking relative to that obtained with 308 nm excitation was achieved.
IT **177601-16-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(bromouridine-enhanced nucleoprotein photocrosslinking with possible involvement of excited tyrosine of protein)
RN 177601-16-0 CAPLUS
CN Benzenepropanamide, α-(acetylamino)-N-ethyl-4-hydroxy-3-(1,2,3,4-tetrahydro-2,4-dioxo-1-β-D-ribofuranosyl-5-pyrimidinyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:711245 CAPLUS
DN 126:75169
TI Preparation of zinc organometallics derived from nucleosides and **nucleic acid** bases and Pd(0) catalyzed coupling with aryl iodides
AU Stevenson, Thomas M.; Prasad, A. S. Bhanu; Citineni, Janakiram Rao; Knochel, Paul
CS Fachbereich Chemie, Philipps-Univ. Marburg, Marburg, D-35032, Germany
SO Tetrahedron Letters (1996), 37(46), 8375-8378
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier
DT Journal
LA English
OS CASREACT 126:75169
AB 5-Iodouracils and 6-iodopurines readily insert zinc dust (25 °C or 70 °C) in THF or N,N-dimethylacetamide (DMAC) affording zincated nucleobases which undergo efficient palladium catalyzed cross-coupling reactions with aryl iodides in good yields. This reaction sequence has been extended to two nucleosides.
IT **185386-81-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of zinc organometallics derived from nucleosides and **nucleic acid** bases and pd catalyzed coupling with aryl iodides)
RN 185386-81-6 CAPLUS
CN Uridine, 3-methyl-5-[3-(trifluoromethyl)phenyl]-, 2',3',5'-triacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:323734 CAPLUS
DN 125:29148
TI Mechanistic Studies of the 5-Iodouracil Chromophore Relevant to Its Use in

Nucleoprotein Photo-Crosslinking

AU Norris, Christopher L.; Meisenheimer, Poncho L.; Koch, Tad H.
CS Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO, 80309-0215, USA

SO Journal of the American Chemical Society (1996), 118(24), 5796-5803
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English

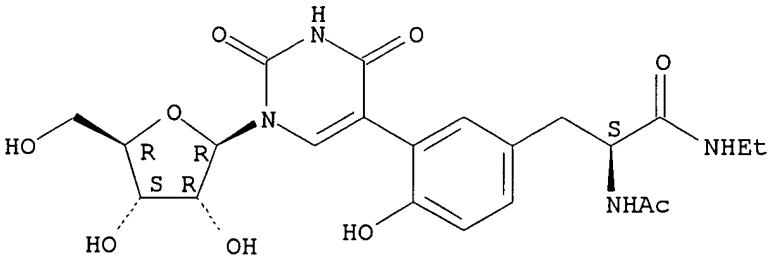
AB The photoreactivity of the 5-iodouracil chromophore was investigated toward understanding photocrosslinking of nucleic acids bearing the chromophore to functionality in associated proteins. Irradiation of 5-iodouridine (IU) in the presence of a 10-fold excess of N-acetyltyrosine N-ethylamide (1) at 308 nm with a XeCl excimer laser or at 325 nm with a HeCd laser yields uridine (U) and N-acetyl-m-(5-uridinyl)tyrosine N-ethylamide (2) in a 1:2 mol ratio. In the presence of N-acetylphenylalanine N-ethylamide, uridine and analogous ortho, meta, and para regioisomeric adducts (3o, 3m, and 3p) were formed in a similar U to adduct mole ratio. The primary photochem. process leading to products was established as carbon-iodine bond homolysis in the first excited singlet state from a deuterium labeling experiment, photoacoustic calorimetry, and quantum yield measurements. Photoredn. of IU in 2-propanol-d solvent gave U with no deuterium incorporation. Photoacoustic calorimetric measurements established that triplet benzophenone transferred energy to IU with a rate constant of 2 + 109 M-1 s-1. Further, the reaction of IU with 1 to form 2 was sensitized by benzophenone; however, comparison of quantum yields upon direct and sensitized excitation indicated that, at most, only a small portion of the reactions occurred via the triplet state. With direct excitation of IU, quantum yields as a function of the concentration of 1 showed that U and adduct 2 resulted from a common intermediate proposed to be the 5-uridinyl radical. Uridine formation was enhanced by the presence of hydrogen atom donors at the expense of formation of 2. Quantum yields were independent of excitation wavelength in the region 310-330 nm but not the reaction medium. The quantum yield of uridine formation but not adduct formation was approx. an order of magnitude higher in 90% acetonitrile-10% water than in pH 7 water. The results are discussed in terms of high-yield crosslinking of nucleic acids bearing the 5-iodouracil chromophore to associated proteins in light of cocrystal x-ray structural data.

IT **177601-16-0 177601-17-1 177601-18-2 177601-19-3**
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative) (mechanistic studies of 5-iodouracil chromophore relevant to its use in nucleoprotein photocrosslinking)

RN 177601-16-0 CAPLUS

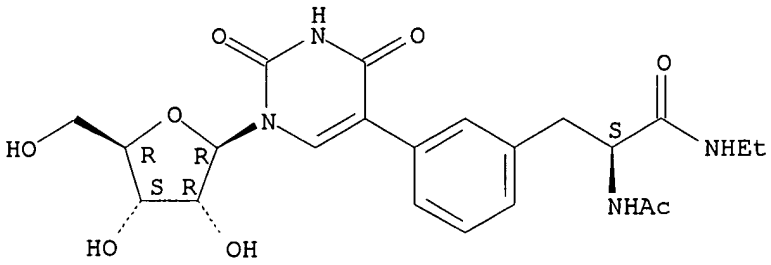
CN Benzenepropanamide, α-(acetylamino)-N-ethyl-4-hydroxy-3-(1,2,3,4-tetrahydro-2,4-dioxo-1-β-D-ribofuranosyl-5-pyrimidinyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



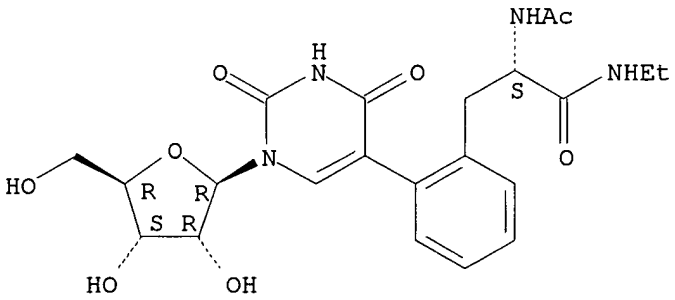
RN 177601-17-1 CAPLUS
CN Benzenepropanamide, α-(acetylamino)-N-ethyl-3-(1,2,3,4-tetrahydro-2,4-dioxo-1-β-D-ribofuranosyl-5-pyrimidinyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



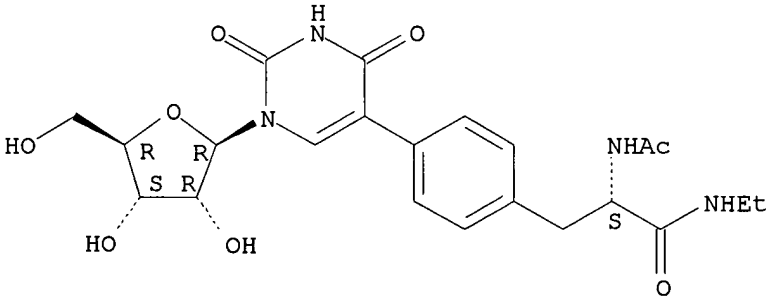
RN 177601-18-2 CAPLUS
CN Benzenepropanamide, α-(acetylamino)-N-ethyl-2-(1,2,3,4-tetrahydro-2,4-dioxo-1-β-D-ribofuranosyl-5-pyrimidinyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 177601-19-3 CAPLUS
CN Benzenepropanamide, α-(acetylamino)-N-ethyl-4-(1,2,3,4-tetrahydro-2,4-dioxo-1-β-D-ribofuranosyl-5-pyrimidinyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:931223 CAPLUS
DN 124:30268
TI Preparation of binding competent oligomers containing unsaturated 3',5'

and 2',5' linkages and related compounds.
IN Matteucci, Mark D.; Cao, Xiaodong
PA Gilead Sciences, Inc., USA
SO PCT Int. Appl., 123 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 3

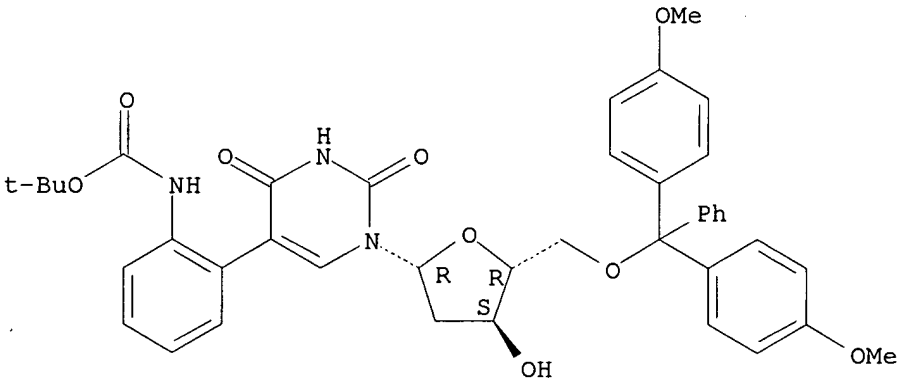
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9511911	A1	19950504	WO 1994-US12202	19941025
	W: CA, JP, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	US 5434257	A	19950718	US 1993-142785	19931026
PRAI	US 1993-142785	A	19931026		
	US 1992-892902	A2	19920601		

AB Oligomers having ≥1 substitute linkage of the form 2'/3' -O-CH2-CH: 5' or 3' -S-CH2-CH: 5' between adjacent nucleomonomers, and related compds., are disclosed. The oligonucleotide analogs are easy to synthesize, stable in vivo, resistant to endogenous nucleases and are able to hybridize to target **nucleic acid** sequences in a sequence specific manner. Thus, 5' TCTCTCTCTCT#TT#TT 3' (# = 3' allyl sulfide linkage; C = 5-methylcytidine) showed a ΔTm/sub. = -1.50° for binding to a single stranded RNA target.

IT **169243-63-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of binding competent oligomers containing unsatd. 3',5' and 2',5'
linkages and related compds.)

RN 169243-63-4 CAPLUS
CN Carbamic acid, [2-[1-[5-O-[bis(4-methoxyphenyl)phenylmethyl]-2-deoxy-β-D-erythro-pentofuranosyl]-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:871986 CAPLUS
DN 123:314400
TI Preparation of fused pyrimidine derivatives as fluorescence-labeled binding partners for oligodeoxyribonucleotides
IN Matteucci, Mark D.; Jones, Robert J.; Lin, Kuei-Ying
PA Gilead Sciences, Inc., USA
SO PCT Int. Appl., 75 pp.
CODEN: PIXXD2

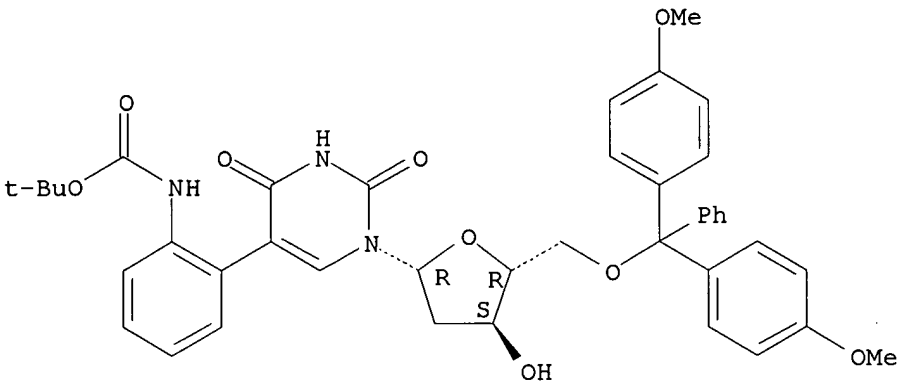
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9507918	A2	19950323	WO 1994-US10536	19940916
	WO 9507918	A3	19950803		
	W: JP				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	US 5502177	A	19960326	US 1993-123505	19930917
	EP 719272	A1	19960703	EP 1994-929830	19940916
	EP 719272	B1	20030507		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	JP 09506859	T2	19970708	JP 1994-509393	19940916
	AT 239752	E	20030515	AT 1994-929830	19940916
	US 6005096	A	19991221	US 1995-436991	19950508
	US 5763588	A	19980609	US 1995-481719	19950607
	US 6617437	B1	20030909	US 1999-468454	19991221
	US 2003207824	A1	20031106	US 2002-294066	20021114
PRAI	US 1993-123505	A	19930917		
	WO 1994-US10536	W	19940916		
	US 1995-436991	A1	19950508		
	US 1999-468454	A1	19991221		

OS MARPAT 123:314400
GI For diagram(s), see printed CA Issue.
AB Fused pyrimidine compds. [I; R1 = a binding partner, a linker, H; a, b = 0 or 1 and a + b = 0 or 1; A = N or C; X = S, O, CO, NH, NCH2R6; Y = CO; Z is taken together with A to form an aryl or heteroaryl ring structure comprising 5 or 6 ring atoms wherein the heteroaryl ring comprises a single O ring heteroatom, a single N ring heteroatom, a single S ring heteroatom, a single O and a single N ring heteroatom separated by a carbon atom, a single S and a single N ring heteroatom separated by a carbon atom 2 N ring heteroatoms separated by a carbon atom, or 2 N ring heteroatoms at least two of which are separated by a carbon atom, and wherein the aryl or heteroaryl ring carbon atoms are unsubstituted with other than H or at least 1 nonbridging ring carbon atom is substituted with R6 or oxo; R6 = H, C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, NO2, (un)protected NH2, cyano, halo; an R6 is taken together with an adjacent R6 to complete a ring containing 5 or 6 ring atoms; provided that when a = 0 and b = 1, and R1 = Q; wherein D2 = (un)protected OH, mono-, di- or triphosphate, or an oligodeoxyribonucleotide otherwise containing only the bases A, G, T and C; D3 = H or OH; then Z ≠ unsubstituted Ph], useful as therapeutics and labels in diagnostics, are prepared These compds. increase the hybridization affinity of oligonucleotides for their complementary sequences, provide improved detectable labels for use in diagnostic assays, enhance diagnostic assays which employ oligonucleotides, and also improve the therapeutic efficacy of oligonucleotides. Thus, 5-iodo-2'-deoxyuridine was condensed with N-tert-butoxylcarbonyl-2-(trimethylstannyl)aniline in the presence of (Ph3P)2PdCl2 in DMF at 50°, followed by tritylation with dimethoxytrityl chloride in pyridine at 20° for 1 h, to give 5-(2-N-tert-butoxycarbonylanilino)-5'-dimethoxytrityl-2'-deoxyuridine, which was cyclized by treatment with (1) Me3SiNMe2 in MeCN at 20° for 2 h, (2) mesitylenesulfonyl chloride and 4-dimethylaminopyridine in MeCN at 20° for 4 h, (3) DBU for 30 min at 20°, and (4) H2O for 1 h to give a benzopyrimidine tricyclic nucleoside (II; X = bond, R = H, DMT = 4,4'-dimethoxytrityl). Other tricyclic pyrimidine nucleosides II (X = O, S; R = H) and a tetracyclic pyrimidine nucleoside (III) were also prepared, converted into its 3' hydrogen phosphonate derivative, e.g. II [R = PH(O)O-.Et3N+H], and incorporated into oligonucleotides by standard procedures (no details given). The oligonucleotides containing fused pyrimidine nucleosides I showed enhanced RNA affinity.

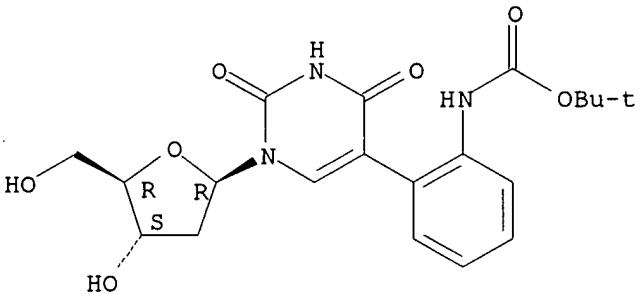
IT **169243-63-4P 169243-64-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of fused pyrimidine nucleoside derivs. as intermediates for fluorescence-labeled oligodeoxyribonucleotides in diagnostics and therapeutics)
RN 169243-63-4 CAPLUS
CN Carbamic acid, [2-[1-[5-O-[bis(4-methoxyphenyl)phenylmethyl]-2-deoxy-β-D-erythro-pentofuranosyl]-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 169243-64-5 CAPLUS
CN Carbamic acid, [2-[1-(2-deoxy-β-D-erythro-pentofuranosyl)-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:759132 CAPLUS
DN 124:146760
TI Oligonucleotide analogs containing unsaturated 3',5' and 2',5' allyl ether and allyl sulfide linkages capable of hybridizing to target **nucleic acid** sequences
IN Matteucci, Mark D.; Cao, Xiaodong
PA Gilead Sciences, Inc., USA
SO U.S., 77 pp. Cont.-in-part of U.S. Ser. No. 892,902.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 3

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

PI	US 5434257	A	19950718	US 1993-142785	19931026
	US 5817781	A	19981006	US 1992-892902	19920601
	AT 174599	E	19990115	AT 1993-915177	19930601
	WO 9511911	A1	19950504	WO 1994-US12202	19941025
	W: CA, JP, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	US 6410702	B1	20020625	US 1998-165883	19981002
	US 2003120050	A1	20030626	US 2002-176763	20020621
	US 6683166	B2	20040127		
PRAI	US 1992-892902	A2	19920601		
	US 1993-142785	A	19931026		
	US 1998-165883	A1	19981002		

OS MARPAT 124:146760

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Oligonucleotide analogs I and II where X is S, O, CH2, CHF or CF2 ; X1 is O or S; R1 is independently H, an oligomer or a blocking group including PO3-2, O-dimethoxytrityl (DMTO), O-monomethoxytrityl (MMTO), H-phosphonate (OPO2H), methylphosphonate (OPO3CH3), methylphosphonamidite, or a phosphoramidite such as β-cyanoethylphosphoramidite; R2 independently is O-alkyl (C1-C12 including O-Me, O-Et, O-Pr, O-Bu and their isomers), S-alkyl(C1-C12), H, OH, OCH3, SCH3, OCH2CH:CH2 (O-allyl), OC3H7 (O-propyl), SCH2CHCH2, or a halogen (F, Cl, Br or I); B is independently a base, and n is 0-100, preferably 0-28; both R1 taken together can comprise a circular oligomer and may be covalently linked, for example, at a terminal 5' position with a terminal 2' or 3' position, are disclosed. The substitute linkage replace the usual phosphodiester linkage found in unmodified nucleic acids. The oligonucleotide analogs are easy to synthesize, stable in vivo, resistant to endogenous nucleases and are able to hybridize to target **nucleic acid** sequences in a sequence specific manner. Thus, e.g., 3'-H-phosphonate dimers III (X = O, S, preparation given) were incorporated into oligomers (5' TCT CTC TCT CT#T T#TT 3'; # = X-containing linkage) and tested for binding to single stranded DNA (3' AGA GAG AGA GAA AAA 5'): ΔTm was -3.25 and -3.0°, resp., for X = O and X = S.

IT **169243-63-4P**

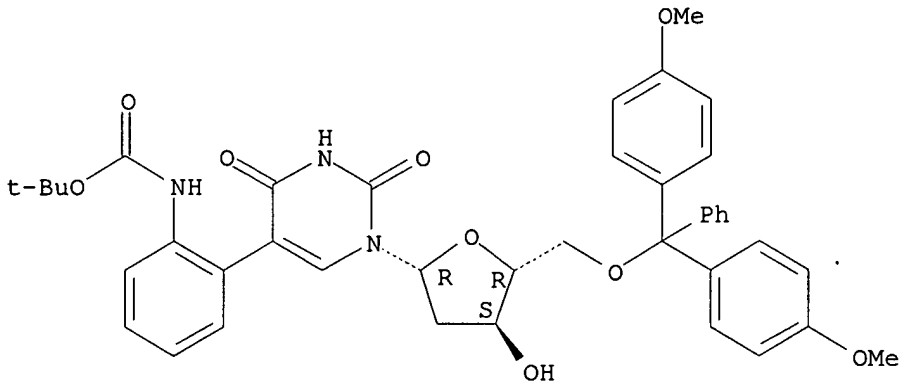
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(oligonucleotide analogs containing unsatd. 3',5' and 2',5' allyl ether and allyl sulfide linkages capable of hybridizing to target **nucleic acid** sequences)

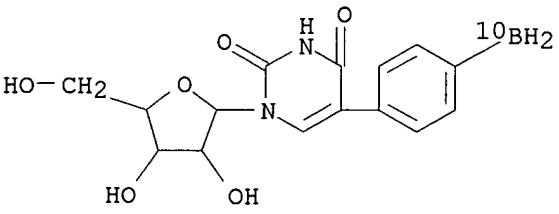
RN 169243-63-4 CAPLUS

CN Carbamic acid, [2-[1-[5-O-[bis(4-methoxyphenyl)phenylmethyl]-2-deoxy-β-D-erythro-pentofuranosyl]-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1992:647824 CAPLUS
DN 117:247824
TI Enhancement of thermal neutron induced killing effect on HeLa cells containing boron-10 **nucleic acid** derivatives
AU Ujeno, Y.; Akaboshi, M.; Akuta, K.; Maki, T.; Kawai, K.; Yamamoto, Y.
CS Res. React. Inst., Kyoto Univ., Osaka, 590-04, Japan
SO Prog. Neutron Capture Ther. Cancer, [Proc. Int. Symp.], 4th (1992), Meeting Date 1990, 349-51. Editor(s): Allen, Barry J.; Moore, Douglas E.; Harrington, Baiba V. Publisher: Plenum, New York, N. Y.
CODEN: 58COA3
DT Conference
LA English
AB The present study deals with the enhanced killing of HeLa S3 cells containing boron-10 nucleic acids in vitro by irradiation in the thermal neutron beam of the Kyoto University Reactor (KUR). The enhancement was measured by the changes in 4 radiobiol. parameters.
IT **144601-99-0**
RL: BIOL (Biological study)
(neutron lethality to HeLa cells enhancement by)
RN 144601-99-0 CAPLUS
CN Uridine, 5-[4-(boryl-10B)phenyl]- (9CI) (CA INDEX NAME)



L6 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1981:192661 CAPLUS
DN 94:192661
TI Organic chemical approach to photo-cross-links of nucleic acids to proteins
AU Matsuura, Teruo; Saito, Isao; Ito, Satoru; Sugiyama, Hiroshi; Shinmura, Tetsuya
CS Dep. Synth. Chem., Kyoto Univ., Kyoto, 606, Japan
SO Pure and Applied Chemistry (1980), 52(12), 2705-15
CODEN: PACHAS; ISSN: 0033-4545
DT Journal
LA English

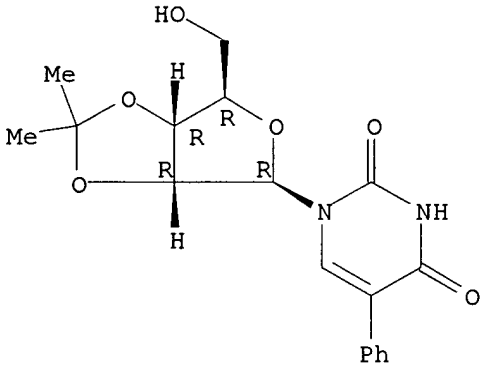
AB Model systems for the photochem. crosslinkage of nucleic acids to proteins were studied. 5-Bromouracil and its derivs. underwent selective photocoupling to tryptophan, indoles, and electron-rich aromatic compds. under various irradiation conditions. Four types of reaction mechanism were observed: triplet coupling of bromouracils, a double electron transfer in the presence of an electron carrier, mixed aggregate formation in aqueous frozen solution, and fluorescence quenching of the aroms. by bromouracil. The stereochem. of photocoupling was studied by examination of the spectral an photochem. behavior of 8 of tryptophan-pyrimidine base derivs., and the photoreactions of other bases to amino acids is reported.

IT **75759-65-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

RN 75759-65-8 CAPLUS

CN Uridine, 2',3'-O-(1-methylethylidene)-5-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

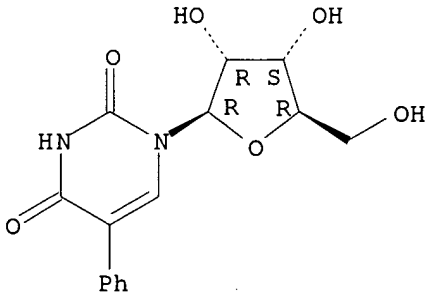


IT **75759-66-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 75759-66-9 CAPLUS

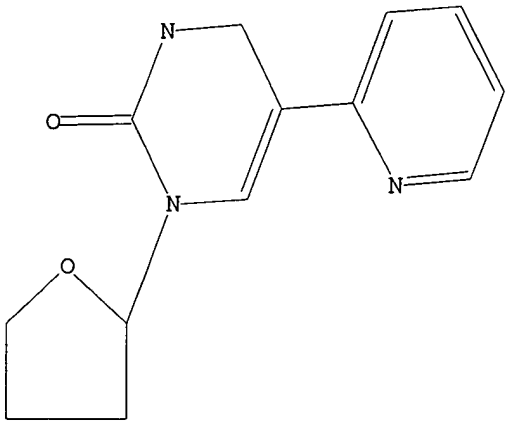
CN Uridine, 5-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=>

```
 * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:04:16 ON 28 DEC 2004

=> file reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         0.21       0.21

FILE 'REGISTRY' ENTERED AT 10:04:26 ON 28 DEC 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   26 DEC 2004  HIGHEST RN 802853-20-9
DICTIONARY FILE UPDATES:  26 DEC 2004  HIGHEST RN 802853-20-9

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

*** YOU HAVE NEW MAIL ***

=>
Uploading C:\Program Files\Stnexp\Queries\107306433.str

L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR
```




```
Structure attributes must be viewed using STN Express query preparation.
```

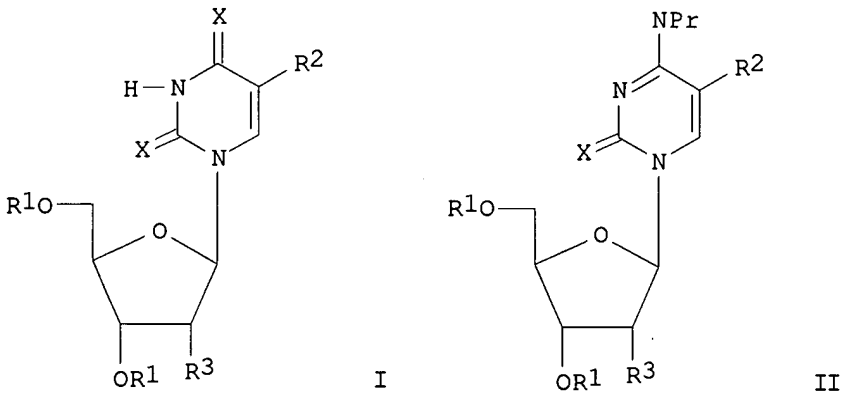
```
=> s l1 full
FULL SEARCH INITIATED 10:04:48 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     78 TO ITERATE

100.0% PROCESSED      78 ITERATIONS                              7 ANSWERS
SEARCH TIME: 00.00.01

L2            7 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   155.42     155.63

FILE 'CAPLUS' ENTERED AT 10:04:52 ON 28 DEC 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)
```



```
FILE COVERS 1907 - 28 Dec 2004  VOL 142 ISS 1
FILE LAST UPDATED: 24 Dec 2004  (20041224/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.

*** YOU HAVE NEW MAIL ***

=> s l2
L3            6 L2

=> d l3 bib abs hitstr 1-6

L3   ANSWER 1 OF 6  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   1997:456106  CAPLUS
DN   127:190987
TI   Enhanced triple-helix and double-helix formation with
     oligodeoxyribonucleotides containing modified pyrimidines
IN   Froehler, Brian; Wagner, Rick; Matteucci, Mark; Jones, Robert J.;
     Gutierrez, Arnold J.; Pudlo, Jeff
PA   Gilead Sciences, Inc., USA
SO   U.S., 104 pp., Cont.-in-part of U.S. Ser. No. 965,941, abandoned.
     CODEN: USXXAM
DT   Patent
LA   English
FAN.CNT 2
     PATENT NO.          KIND   DATE        APPLICATION NO.         DATE
     --------------      ----   --------    --------------------    --------
PI   US 5645985           A     19970708    US 1992-976103          19921125
     US 5484908           A     19960116    US 1991-799824          19911126
```

	EP 1256589	A2	20021113	EP 2002-13297	19921124
	EP 1256589	A3	20030917		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
	TW 393513	B	20000611	TW 1993-82101747	19930308
	AU 9463453	A1	19940915	AU 1994-63453	19940601
	AU 679508	B2	19970703		
	US 6235887	B1	20010522	US 1994-338352	19941114
	US 5830653	A	19981103	US 1995-473481	19950607
	US 6380368	B1	20020430	US 1996-599738	19960212
	US 2003096980	A1	20030522	US 2001-24818	20011218
	US 2003170680	A1	20030911	US 2002-294203	20021114
	US 2004220395	A1	20041104	US 2003-730643	20031208
PRAI	US 1991-799824	A2	19911126		
	US 1992-935444	B2	19920825		
	US 1992-965941	B2	19921023		
	EP 1993-900636	A3	19921124		
	US 1992-976103	A	19921125		
	US 1994-338352	A1	19941114		
	US 1996-599738	A3	19960212		
	US 2001-24818	A1	20011218		
	US 2002-294203	A3	20021114		
OS	MARPAT 127:190987				

GI



I II

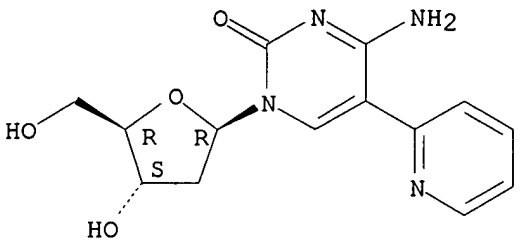
AB Nucleomonomer nucleosides I and II [X = O, S; R1 = H, blocking group; H-phosphonate, phosphoramidite, alkylphosphonamidite; R2 = (un)substituted alkenyl or alkynyl, alkynylheteroaryl; Pr = (H)2 or protecting group; R3 = H, OH, F, OMe, OEt, SMe, SEt] were prepared and incorporated into DNA duplexes and triplexes. Novel oligodeoxyribonucleotides are disclosed which have enhanced ability with respect to forming duplexes or triplexes compared with oligomers containing only conventional bases. The oligomers contain the bases 5-(1-propynyl)uracil, 5-(1-propynyl)cytosine or related analogs. The oligomers of the invention are capable of (i) forming triplexes with various target sequences such as virus or oncogene sequences by coupling into the major groove of a target DNA duplex at physiol. pH or (ii) forming duplexes by binding to single-stranded DNA or to RNA encoded by target genes. The oligomers of the invention can be constructed to have any desired sequence, provided the sequence normally includes one or more bases that is replaced with the analogs of the invention. Compns. of the invention can be used used for diagnostic purposes in order to detect viruses or disease conditions. Thus, 5-propynyl-2'-O-allyluridine was prepared and incorporated into DNA duplexes

and triplexes.

IT **143325-17-1P 151091-78-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enhanced triple-helix and double-helix formation with oligodeoxyribonucleotides containing modified pyrimidines)

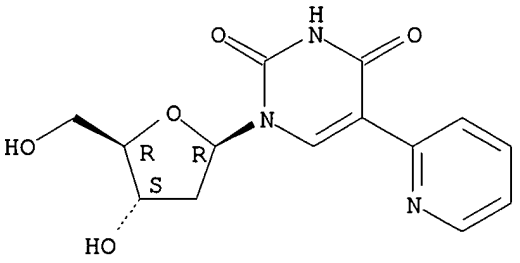
RN 143325-17-1 CAPLUS
CN Cytidine, 2'-deoxy-5-(2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 151091-78-0 CAPLUS
CN Uridine, 2'-deoxy-5-(2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:631025 CAPLUS
DN 123:74138
TI Substrate specificities of mitochondrial thymidine kinase and cytosolic deoxycytidine kinase against 5-aryl substituted pyrimidine-2'-deoxyribose analogs
AU Eriksson, Staffan; Wang, Jianghai; Gronowitz, Salo; Johansson, Nils Gunnar
CS Department Veterinary Medical Chemistry, Swedish University Agricultural Sciences, Uppsala, S-75123, Swed.
SO Nucleosides & Nucleotides (1995), 14(3-5), 507-10
CODEN: NUNUD5; ISSN: 0732-8311
PB Dekker
DT Journal
LA English
AB Some 5-aryl-2'-deoxyuridine and -deoxycytidine analogs, many with known antiviral activity, were evaluated as substrates for pure deoxycytidine kinase (dCK) and pure mitochondrial thymidine kinase (TK2). Some of the deoxyuridine compds. were also tested with pure cytosolic thymidine kinase (TK1). TK2 showed the highest phosphorylation activity with this type of analogs.

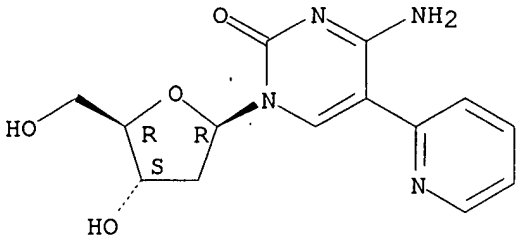
IT **143325-17-1**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(substrate specificities of cytosolic and mitochondrial thymidine

kinase and cytosolic deoxycytidine kinase against 5-aryl substituted pyrimidine-2'-deoxyribose analogs)

RN 143325-17-1 CAPLUS

CN Cytidine, 2'-deoxy-5-(2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1994:436104 CAPLUS

DN 121:36104

TI 5-Heteroaryl-2'-deoxyuridine Analogs. Synthesis and Incorporation into High-Affinity Oligonucleotides

AU Gutierrez, Arnold J.; Terhorst, Terry J.; Matteucci, Mark D.; Froehler, Brian C.

CS Gilead Sciences Inc., Foster City, CA, 94404, USA

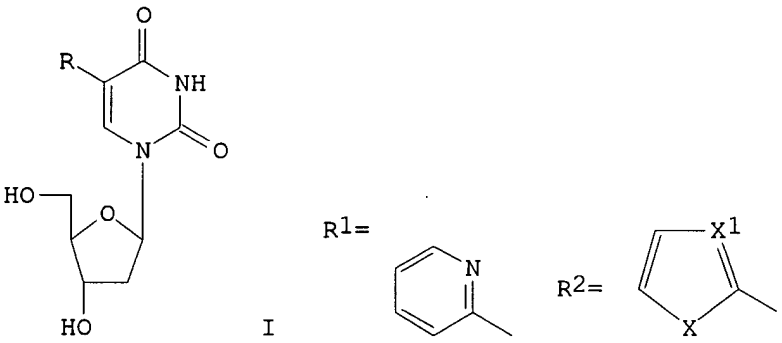
SO Journal of the American Chemical Society (1994), 116(13), 5540-4
CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA English

OS CASREACT 121:36104

GI



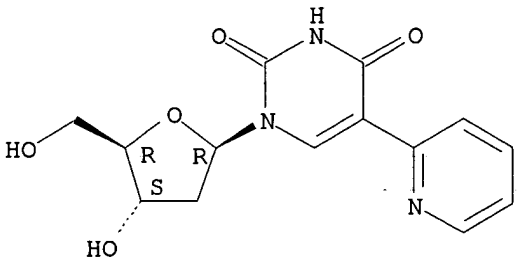
AB C-5 heteroaryl-2'-deoxyuridines I (R = R1, R2;X = S, X1 = CH, N; X = NH, X1 = N), were synthesized from 5-iodo-2'-deoxyuridine. Palladium-catalyzed coupling with heteroarylstannanes proved to be a convenient and general method of preparation Oligonucleotides containing I gave enhanced thermal stability to complementary RNA relative to thymidine. Thermal denaturation studies showed that oligodeoxynucleotides (ODNs) containing 5-(thiazol-2-yl)-2'-deoxyuridine exhibit the highest thermal denaturation (Tm) and therefore may increase the potency of these ODNs to inhibit gene expression in a sequence-specific manner.

IT **151091-78-0P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and incorporation of, into oligodeoxyribonucleotide duplex RNA)

RN 151091-78-0 CAPLUS
CN Uridine, 2'-deoxy-5-(2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1993:642931 CAPLUS
DN 119:242931
TI Enhanced triple- and double-helix formation with oligomers containing modified pyrimidines
IN Froehler, Brian; Wagner, Rick; Matteucci, Mark; Jones, Robert J.; Gutierrez, Arnold J.; Pudlo, Jeff
PA Gilead Sciences, Inc., USA
SO PCT Int. Appl., 170 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9310820	A1	19930610	WO 1992-US10115	19921124
	W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, PL, PT, RO, RU, SD, SE				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
	US 5484908	A	19960116	US 1991-799824	19911126
	AU 9332227	A1	19930628	AU 1993-32227	19921124
	EP 637965	A1	19950215	EP 1993-900636	19921124
	EP 637965	B1	20021016		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	JP 07501527	T2	19950216	JP 1992-509622	19921124
	EP 1256589	A2	20021113	EP 2002-13297	19921124
	EP 1256589	A3	20030917		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
	AT 226093	E	20021115	AT 1993-900636	19921124
	AU 9463453	A1	19940915	AU 1994-63453	19940601
	AU 679508	B2	19970703		
	US 6235887	B1	20010522	US 1994-338352	19941114
	US 2003096980	A1	20030522	US 2001-24818	20011218
	US 2003170680	A1	20030911	US 2002-294203	20021114
PRAI	US 1991-799824	A	19911126		
	US 1992-935444	A	19920825		
	US 1992-965941	A	19921023		
	EP 1993-900636	A3	19921124		
	WO 1992-US10115	A	19921124		
	US 1996-599738	A3	19960212		
	US 2001-24818	A1	20011218		

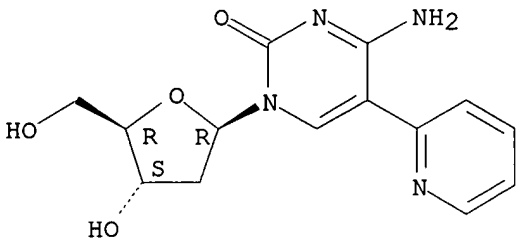
AB The modified pyrimidines such as 5-(1-propynyl)uracil or 5-(1-propynyl)cytosine are prepared by substitution at the 5-position. Hybridized with double- and single-stranded nucleic acids, resp., the

oligonucleotides containing the modified pyrimidines have enhanced formation of triple- and double-helix structures. The oligonucleotides are useful as pharmaceuticals for treatment of virus-associated diseases, for detection of double- or single-stranded nucleic acids, for amplification of nucleic acids, and for inhibition of target gene expression. Preparation of 5-(1-propynyl)-2'-deoxyuridine H-phosphonate and oligonucleotides containing the 5-propynyl uracil, and the enhanced formation of triple- and double-helix structures with the oligonucleotides were shown.

IT **143325-17-1 151091-78-0**
RL: USES (Uses)
(oligonucleotides containing, for enhanced formation of triple- and double-helix for treatment of virus-associated diseases)

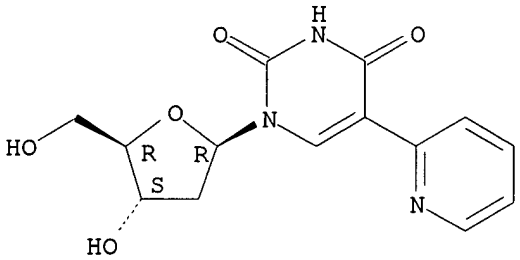
RN 143325-17-1 CAPLUS
CN Cytidine, 2'-deoxy-5-(2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 151091-78-0 CAPLUS
CN Uridine, 2'-deoxy-5-(2-pyridinyl)- (9CI) (CA INDEX NAME)

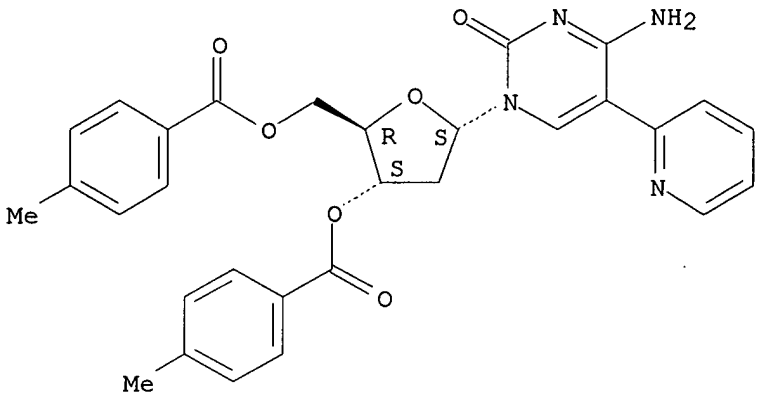
Absolute stereochemistry.



L3 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1992:531487 CAPLUS
DN 117:131487
TI Synthesis and antiviral activity of various 5-substituted 2'-deoxyuridines and -cytidines
AU Peters, Dan; Hoernfeldt, Anna Britta; Gronowitz, Salo; Johansson, Nils Gunnar
CS Chem. Cent., Lund, S-221 00, Swed.
SO Nucleosides & Nucleotides (1992), 11(6), 1151-73
CODEN: NUNUD5; ISSN: 0732-8311
DT Journal
LA English
AB 5-Cyclopropyl-2'-deoxycytidine and some 5-aryl-2'-deoxyuridines and -cytidines have been prepared and their inhibition of HIV have been tested.
IT **143324-91-8P 143324-92-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deblocking of)

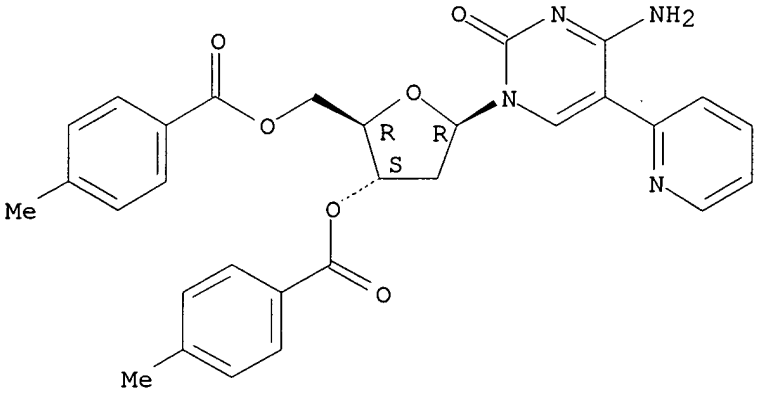
RN 143324-91-8 CAPLUS
CN 2(1H)-Pyrimidinone, 4-amino-1-[2-deoxy-3,5-bis-O-(4-methylbenzoyl)-α-D-erythro-pentofuranosyl]-5-(2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



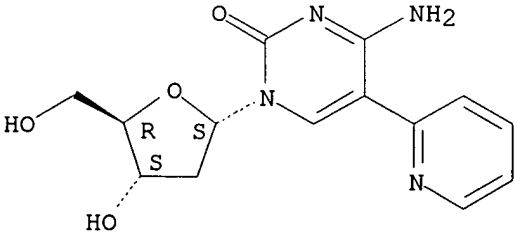
RN 143324-92-9 CAPLUS
CN Cytidine, 2'-deoxy-5-(2-pyridinyl)-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



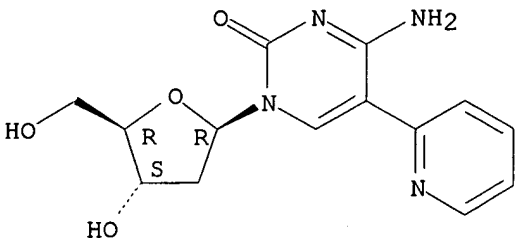
IT **143325-16-0P 143325-17-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 143325-16-0 CAPLUS
CN 2(1H)-Pyrimidinone, 4-amino-1-(2-deoxy-α-D-erythro-pentofuranosyl)-5-(2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 143325-17-1 CAPLUS
CN Cytidine, 2'-deoxy-5-(2-pyridinyl)- (9CI) (CA INDEX NAME)

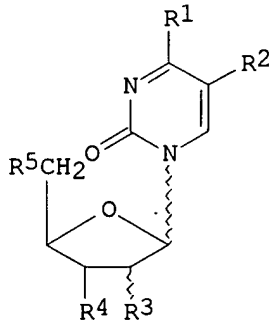
Absolute stereochemistry.



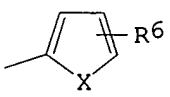
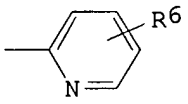
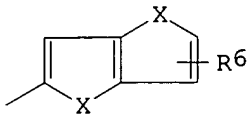
L3 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:235778 CAPLUS
DN 112:235778
TI Preparation of pyrimidine nucleosides as virucides and their intermediates
IN Johansson, K. Nils Gunnar; Malmberg, Hans C. G.; Noreen, Rolf; Sahlberg, S. Christer; Sohn, Daniel D.; Gronowitz, Salo
PA Medivir AB, Swed.
SO PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 8912061	A1	19891214	WO 1989-SE322	19890607
	W: AU, DK, FI, HU, JP, KR, NO, US				
	CA 1339313	A1	19970819	CA 1989-601897	19890606
	AU 8937504	A1	19900105	AU 1989-37504	19890607
	AU 637574	B2	19930603		
	EP 357571	A2	19900307	EP 1989-850184	19890607
	EP 357571	A3	19900613		
	EP 357571	B1	19960403		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	JP 03504969	T2	19911031	JP 1989-506227	19890607
	JP 2851094	B2	19990127		
	HU 57230	A2	19911128	HU 1989-4340	19890607
	HU 211736	B	19951228		
	EP 691333	A2	19960110	EP 1995-113626	19890607
	EP 691333	A3	19960214		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	AT 136308	E	19960415	AT 1989-850184	19890607
	ES 2087090	T3	19960716	ES 1989-850184	19890607
	NO 9005300	A	19910206	NO 1990-5300	19901207
	NO 175981	B	19941003		
	NO 175981	C	19950111		
	DK 9002918	A	19910207	DK 1990-2918	19901207
	FI 94643	B	19950630	FI 1990-6053	19901207
	FI 94643	C	19951010		
	US 5440040	A	19950808	US 1991-613900	19910118
	US 5576429	A	19961119	US 1995-395877	19950228
PRAI	SE 1988-2173	A	19880610		
	EP 1989-850184	A3	19890607		
	WO 1989-SE322	A	19890607		
	US 1991-613900	A3	19910118		

OS MARPAT 112:235778
GI



I

Q=  Q1=  Q2= 

AB The title compds. [I; R1 = OH, NH2; R2 = (hetero)aryl, e.g. Q-Q2; X = O, S, Se, (un)substituted NH; R3 = H, OH, F, OMe; R4 = H, F, OH or its ether or ester residue, OMe, cyano, C.tplbond.CH, N3; R5 = OH or its ether or ester residue, (CH2)nP(O)(OM)2, (CH2)nP(O)(OM)CH2P(O)(OM)2; R6 = H, straight or branched C1-10 alkyl, halo, etc.; M = H, a pharmaceutically acceptable counterion; n = 0, 1], useful for treatment of infections by viruses requiring reverse transcriptase for replication, e.g. human immunodeficiency virus (HIV) and hepatitis B virus, were prepared Thus, silylation of 5-(2-thienyl)uracil (II) with hexamethyldisilazane in the presence of Me3SiCl and (NH4)2SO4 under reflux gave bis-trimethylsilylated II which was stirred overnight with 2-deoxy-3,5-di-O-p-toluoyl-D-ribofuranosyl chloride in ClCH2CH2Cl in the presence of mol. sieve 4A. The product was treated with MeONa in MeOH to give α- and β-I (R1 = R4 = R5 = OH, R2 = 2-thienyl, R3 = H). α-I in vitro showed IC50 of 0.05-10 μM against HIV in H9 cells. Analogously prepared and tested were addnl. 26 I. Cellular toxicity of I on H9 and F500 cells and inhibition of enzymes (e.g. HIV reverse transcriptase, hepatitis B virus DNA polymerase, and herpes simplex virus type 2 DNA polymerase) by I were also given.

IT **127235-49-8P**

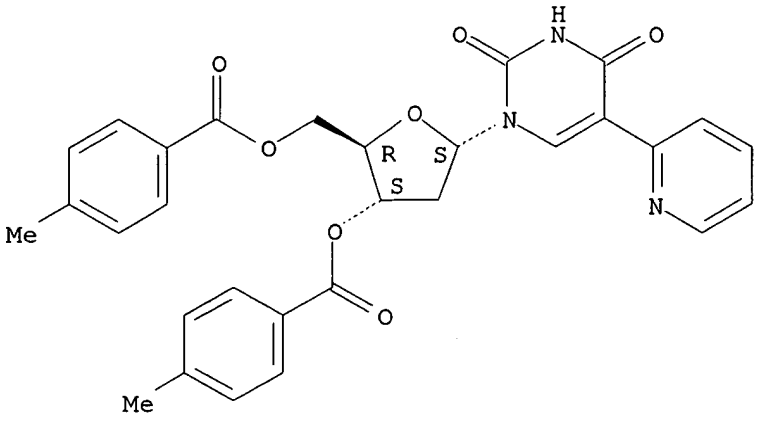
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of pyrimidine nucleoside virucide)

RN 127235-49-8 CAPLUS

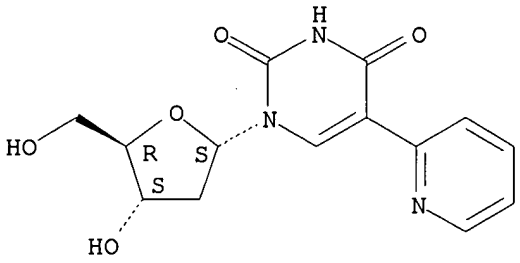
CN 2,4(1H,3H)-Pyrimidinedione, 1-[2-deoxy-3,5-bis-O-(4-methylbenzoyl)-α-D-erythro-pentofuranosyl]-5-(2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



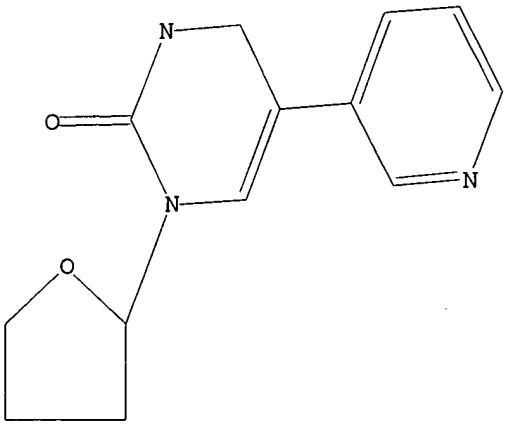
IT **127235-69-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as virucide)
RN 127235-69-2 CAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 1-(2-deoxy-α-D-erythro-pentofuranosyl)-5-(2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=>

```
* * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:07:26 ON 28 DEC 2004

=> file reg
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.21       0.21

FILE 'REGISTRY' ENTERED AT 10:07:34 ON 28 DEC 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   26 DEC 2004  HIGHEST RN 802853-20-9
DICTIONARY FILE UPDATES:  26 DEC 2004  HIGHEST RN 802853-20-9

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

*** YOU HAVE NEW MAIL ***

=>
Uploading C:\Program Files\Stnexp\Queries\107306434.str

L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR
```




```
Structure attributes must be viewed using STN Express query preparation.
```

```
=> s l1 full
FULL SEARCH INITIATED 10:07:56 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    394 TO ITERATE

100.0% PROCESSED     394 ITERATIONS                              8 ANSWERS
SEARCH TIME: 00.00.01

L2             8 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                             155.42     155.63

FILE 'CAPLUS' ENTERED AT 10:08:01 ON 28 DEC 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)


Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.
The CA Lexicon is the copyrighted intellectual property of the
American Chemical Society and is provided to assist you in searching
databases on STN.  Any dissemination, distribution, copying, or storing
of this information, without the prior written consent of CAS, is
strictly prohibited.

FILE COVERS 1907 - 28 Dec 2004  VOL 142 ISS 1
FILE LAST UPDATED: 24 Dec 2004  (20041224/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s l2
L3             6 L2

=> d l3 bib abs histr 1-6
'HISTR' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS --------- GI and AB
ALL --------- BIB, AB, IND, RE
APPS -------- AI, PRAI
BIB --------- AN, plus Bibliographic Data and PI table (default)
CAN --------- List of CA abstract numbers without answer numbers
CBIB -------- AN, plus Compressed Bibliographic Data
DALL -------- ALL, delimited (end of each field identified)
DMAX -------- MAX, delimited for post-processing
FAM --------- AN, PI and PRAI in table, plus Patent Family data
FBIB -------- AN, BIB, plus Patent FAM
IND --------- Indexing data
IPC --------- International Patent Classifications
MAX --------- ALL, plus Patent FAM, RE
PATS -------- PI, SO
SAM --------- CC, SX, TI, ST, IT
SCAN -------- CC, SX, TI, ST, IT (random display, no answer numbers;
```

SCAN must be entered on the same line as the DISPLAY,
e.g., D SCAN or DISPLAY SCAN)
STD --------- BIB, IPC, and NCL

IABS -------- ABS, indented with text labels
IALL -------- ALL, indented with text labels
IBIB -------- BIB, indented with text labels
IMAX -------- MAX, indented with text labels
ISTD -------- STD, indented with text labels

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

HIT --------- Fields containing hit terms
HITIND ------ IC, ICA, ICI, NCL, CC and index field (ST and IT)
containing hit terms
HITRN ------- HIT RN and its text modification
HITSTR ------ HIT RN, its text modification, its CA index name, and
its structure diagram
HITSEQ ------ HIT RN, its text modification, its CA index name, its
structure diagram, plus NTE and SEQ fields
FHITSTR ----- First HIT RN, its text modification, its CA index name, and
its structure diagram
FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
structure diagram, plus NTE and SEQ fields
KWIC -------- Hit term plus 20 words on either side
OCC --------- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of formats include: TI; TI,AU; BIB,ST; TI,IND; TI,SO. You may specify the format fields in any order and the information will be displayed in the same order as the format specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC to view a specified Accession Number.
ENTER DISPLAY FORMAT (BIB):bib

L3 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:871986 CAPLUS
DN 123:314400
TI Preparation of fused pyrimidine derivatives as fluorescence-labeled binding partners for oligodeoxyribonucleotides
IN Matteucci, Mark D.; Jones, Robert J.; Lin, Kuei-Ying
PA Gilead Sciences, Inc., USA
SO PCT Int. Appl., 75 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9507918	A2	19950323	WO 1994-US10536	19940916
	WO 9507918	A3	19950803		
	W: JP				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	US 5502177	A	19960326	US 1993-123505	19930917

	EP 719272	A1	19960703	EP 1994-929830	19940916
	EP 719272	B1	20030507		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	JP 09506859	T2	19970708	JP 1994-509393	19940916
	AT 239752	E	20030515	AT 1994-929830	19940916
	US 6005096	A	19991221	US 1995-436991	19950508
	US 5763588	A	19980609	US 1995-481719	19950607
	US 6617437	B1	20030909	US 1999-468454	19991221
	US 2003207824	A1	20031106	US 2002-294066	20021114
PRAI	US 1993-123505	A	19930917		
	WO 1994-US10536	W	19940916		
	US 1995-436991	A1	19950508		
	US 1999-468454	A1	19991221		

OS MARPAT 123:314400

L3 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:759132 CAPLUS
DN 124:146760
TI Oligonucleotide analogs containing unsaturated 3',5' and 2',5' allyl ether and allyl sulfide linkages capable of hybridizing to target nucleic acid sequences
IN Matteucci, Mark D.; Cao, Xiaodong
PA Gilead Sciences, Inc., USA
SO U.S., 77 pp. Cont.-in-part of U.S. Ser. No. 892,902.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5434257	A	19950718	US 1993-142785	19931026
	US 5817781	A	19981006	US 1992-892902	19920601
	AT 174599	E	19990115	AT 1993-915177	19930601
	WO 9511911	A1	19950504	WO 1994-US12202	19941025
	W: CA, JP, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	US 6410702	B1	20020625	US 1998-165883	19981002
	US 2003120050	A1	20030626	US 2002-176763	20020621
	US 6683166	B2	20040127		
PRAI	US 1992-892902	A2	19920601		
	US 1993-142785	A	19931026		
	US 1998-165883	A1	19981002		

OS MARPAT 124:146760

L3 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:631025 CAPLUS
DN 123:74138
TI Substrate specificities of mitochondrial thymidine kinase and cytosolic deoxycytidine kinase against 5-aryl substituted pyrimidine-2'-deoxyribose analogs
AU Eriksson, Staffan; Wang, Jianghai; Gronowitz, Salo; Johansson, Nils Gunnar
CS Department Veterinary Medical Chemistry, Swedish University Agricultural Sciences, Uppsala, S-75123, Swed.
SO Nucleosides & Nucleotides (1995), 14(3-5), 507-10
CODEN: NUNUD5; ISSN: 0732-8311
PB Dekker
DT Journal
LA English

L3 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1992:531487 CAPLUS
DN 117:131487

TI Synthesis and antiviral activity of various 5-substituted 2'-deoxyuridines and -cytidines
AU Peters, Dan; Hoernfeldt, Anna Britta; Gronowitz, Salo; Johansson, Nils Gunnar
CS Chem. Cent., Lund, S-221 00, Swed.
SO Nucleosides & Nucleotides (1992), 11(6), 1151-73
CODEN: NUNUD5; ISSN: 0732-8311
DT Journal
LA English

L3 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:235778 CAPLUS
DN 112:235778
TI Preparation of pyrimidine nucleosides as virucides and their intermediates
IN Johansson, K. Nils Gunnar; Malmberg, Hans C. G.; Noreen, Rolf; Sahlberg, S. Christer; Sohn, Daniel D.; Gronowitz, Salo
PA Medivir AB, Swed.
SO PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 8912061	A1	19891214	WO 1989-SE322	19890607
	W: AU, DK, FI, HU, JP, KR, NO, US				
	CA 1339313	A1	19970819	CA 1989-601897	19890606
	AU 8937504	A1	19900105	AU 1989-37504	19890607
	AU 637574	B2	19930603		
	EP 357571	A2	19900307	EP 1989-850184	19890607
	EP 357571	A3	19900613		
	EP 357571	B1	19960403		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	JP 03504969	T2	19911031	JP 1989-506227	19890607
	JP 2851094	B2	19990127		
	HU 57230	A2	19911128	HU 1989-4340	19890607
	HU 211736	B	19951228		
	EP 691333	A2	19960110	EP 1995-113626	19890607
	EP 691333	A3	19960214		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	AT 136308	E	19960415	AT 1989-850184	19890607
	ES 2087090	T3	19960716	ES 1989-850184	19890607
	NO 9005300	A	19910206	NO 1990-5300	19901207
	NO 175981	B	19941003		
	NO 175981	C	19950111		
	DK 9002918	A	19910207	DK 1990-2918	19901207
	FI 94643	B	19950630	FI 1990-6053	19901207
	FI 94643	C	19951010		
	US 5440040	A	19950808	US 1991-613900	19910118
	US 5576429	A	19961119	US 1995-395877	19950228
PRAI	SE 1988-2173	A	19880610		
	EP 1989-850184	A3	19890607		
	WO 1989-SE322	A	19890607		
	US 1991-613900	A3	19910118		

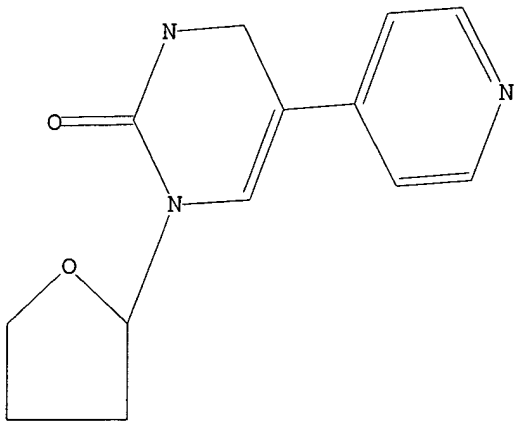
OS MARPAT 112:235778

L3 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1986:130206 CAPLUS
DN 104:130206
TI Diels-Alder reactions of azadienes. A facile approach to the synthesis of pyridine- and pyridazine-substituted pyrimidine nucleosides
AU Maggiora, Linda; Mertes, Mathias P.

CS Dep. Med. Chem., Univ. Kansas, Lawrence, KS, 66045, USA
SO Journal of Organic Chemistry (1986), 51(6), 950-1
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 104:130206

=>

```
* * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:09:39 ON 28 DEC 2004

=> file reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         0.21       0.21

FILE 'REGISTRY' ENTERED AT 10:09:46 ON 28 DEC 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   26 DEC 2004  HIGHEST RN 802853-20-9
DICTIONARY FILE UPDATES:  26 DEC 2004  HIGHEST RN 802853-20-9

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

*** YOU HAVE NEW MAIL ***

=>
Uploading C:\Program Files\Stnexp\Queries\107306435.str

L1      STRUCTURE UPLOADED

=>  d l1
L1 HAS NO ANSWERS
L1              STR
```




```
Structure attributes must be viewed using STN Express query preparation.
```

```
=> s l1 full
FULL SEARCH INITIATED 10:10:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   1070 TO ITERATE

100.0% PROCESSED    1070 ITERATIONS                          7 ANSWERS
SEARCH TIME: 00.00.01

L2            7 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                             155.42     155.63

FILE 'CAPLUS' ENTERED AT 10:10:16 ON 28 DEC 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)
```



```
FILE COVERS 1907 - 28 Dec 2004  VOL 142 ISS 1
FILE LAST UPDATED: 24 Dec 2004  (20041224/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s l2
L3            4 L2

=> d l3 bib abs hitstr 1-4

L3   ANSWER 1 OF 4  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   1995:631025  CAPLUS
DN   123:74138
TI   Substrate specificities of mitochondrial thymidine kinase and cytosolic
     deoxycytidine kinase against 5-aryl substituted pyrimidine-2'-deoxyribose
     analogs
AU   Eriksson, Staffan; Wang, Jianghai; Gronowitz, Salo; Johansson, Nils Gunnar
CS   Department Veterinary Medical Chemistry, Swedish University Agricultural
     Sciences, Uppsala, S-75123, Swed.
SO   Nucleosides & Nucleotides (1995), 14(3-5), 507-10
     CODEN: NUNUD5; ISSN: 0732-8311
PB   Dekker
DT   Journal
LA   English
AB   Some 5-aryl-2'-deoxyuridine and -deoxycytidine analogs, many with known
     antiviral activity, were evaluated as substrates for pure deoxycytidine
     kinase (dCK) and pure mitochondrial thymidine kinase (TK2).  Some of the
     deoxyuridine compds. were also tested with pure cytosolic thymidine kinase
     (TK1).  TK2 showed the highest phosphorylation activity with this type of
```

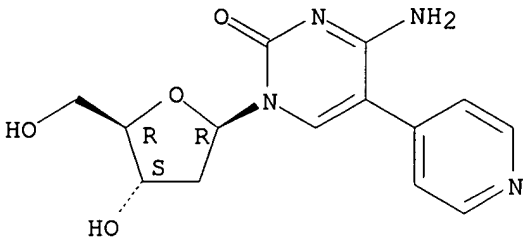
analogs.

IT **143325-21-7**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(substrate specificities of cytosolic and mitochondrial thymidine kinase and cytosolic deoxycytidine kinase against 5-aryl substituted pyrimidine-2'-deoxyribose analogs)

RN 143325-21-7 CAPLUS

CN Cytidine, 2'-deoxy-5-(4-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1992:531487 CAPLUS

DN 117:131487

TI Synthesis and antiviral activity of various 5-substituted 2'-deoxyuridines and -cytidines

AU Peters, Dan; Hoernfeldt, Anna Britta; Gronowitz, Salo; Johansson, Nils Gunnar

CS Chem. Cent., Lund, S-221 00, Swed.

SO Nucleosides & Nucleotides (1992), 11(6), 1151-73
CODEN: NUNUD5; ISSN: 0732-8311

DT Journal

LA English

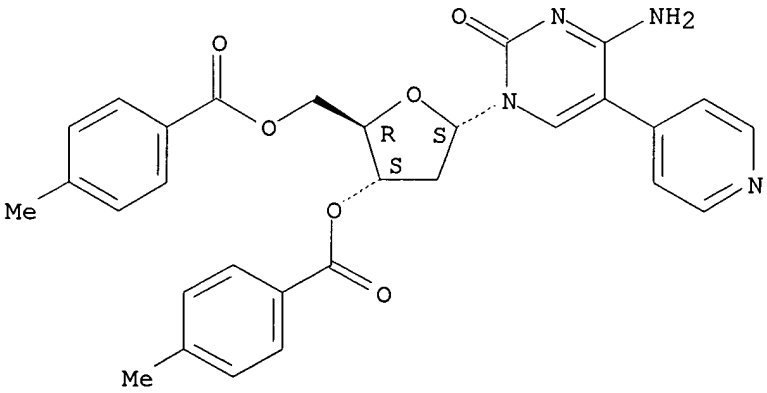
AB 5-Cyclopropyl-2'-deoxycytidine and some 5-aryl-2'-deoxyuridines and -cytidines have been prepared and their inhibition of HIV have been tested.

IT **143324-95-2P 143324-96-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deblocking of)

RN 143324-95-2 CAPLUS

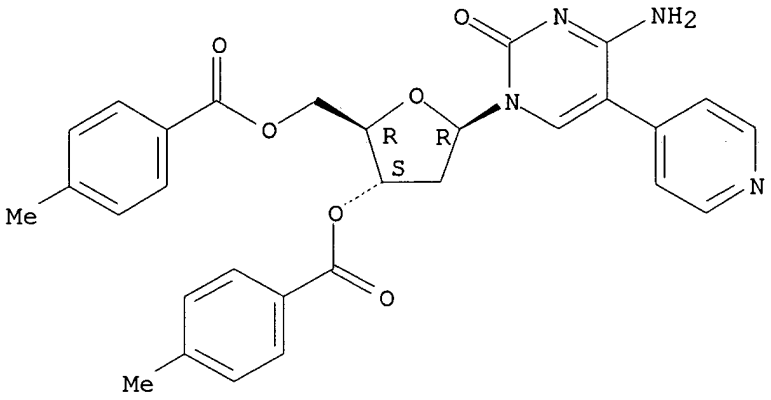
CN 2(1H)-Pyrimidinone, 4-amino-1-[2-deoxy-3,5-bis-O-(4-methylbenzoyl)-α-D-erythro-pentofuranosyl]-5-(4-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



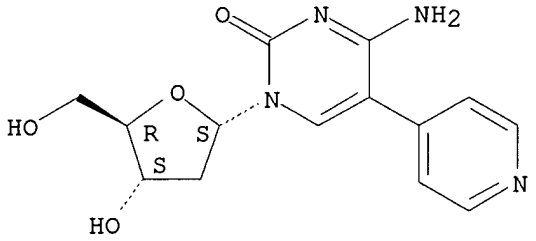
RN 143324-96-3 CAPLUS
CN Cytidine, 2'-deoxy-5-(4-pyridinyl)-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



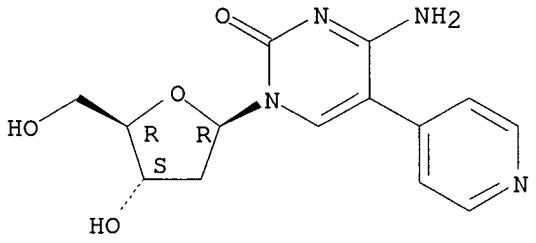
IT **143325-20-6P 143325-21-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 143325-20-6 CAPLUS
CN 2(1H)-Pyrimidinone, 4-amino-1-(2-deoxy-α-D-erythro-pentofuranosyl)-5-(4-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 143325-21-7 CAPLUS
CN Cytidine, 2'-deoxy-5-(4-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

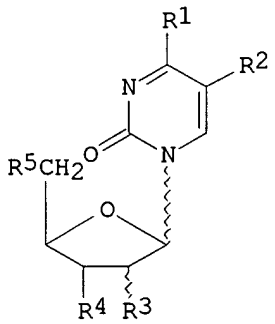


L3 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:235778 CAPLUS
DN 112:235778
TI Preparation of pyrimidine nucleosides as virucides and their intermediates
IN Johansson, K. Nils Gunnar; Malmberg, Hans C. G.; Noreen, Rolf; Sahlberg,

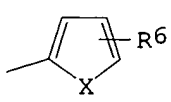
S. Christer; Sohn, Daniel D.; Gronowitz, Salo
PA Medivir AB, Swed.
SO PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

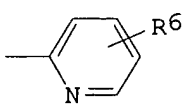
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 8912061	A1	19891214	WO 1989-SE322	19890607
	W: AU, DK, FI, HU, JP, KR, NO, US				
	CA 1339313	A1	19970819	CA 1989-601897	19890606
	AU 8937504	A1	19900105	AU 1989-37504	19890607
	AU 637574	B2	19930603		
	EP 357571	A2	19900307	EP 1989-850184	19890607
	EP 357571	A3	19900613		
	EP 357571	B1	19960403		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	JP 03504969	T2	19911031	JP 1989-506227	19890607
	JP 2851094	B2	19990127		
	HU 57230	A2	19911128	HU 1989-4340	19890607
	HU 211736	B	19951228		
	EP 691333	A2	19960110	EP 1995-113626	19890607
	EP 691333	A3	19960214		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	AT 136308	E	19960415	AT 1989-850184	19890607
	ES 2087090	T3	19960716	ES 1989-850184	19890607
	NO 9005300	A	19910206	NO 1990-5300	19901207
	NO 175981	B	19941003		
	NO 175981	C	19950111		
	DK 9002918	A	19910207	DK 1990-2918	19901207
	FI 94643	B	19950630	FI 1990-6053	19901207
	FI 94643	C	19951010		
	US 5440040	A	19950808	US 1991-613900	19910118
	US 5576429	A	19961119	US 1995-395877	19950228
PRAI	SE 1988-2173	A	19880610		
	EP 1989-850184	A3	19890607		
	WO 1989-SE322	A	19890607		
	US 1991-613900	A3	19910118		

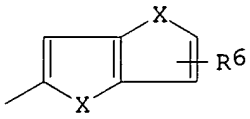
OS MARPAT 112:235778
GI



I

Q= 

Q1= 

Q2= 

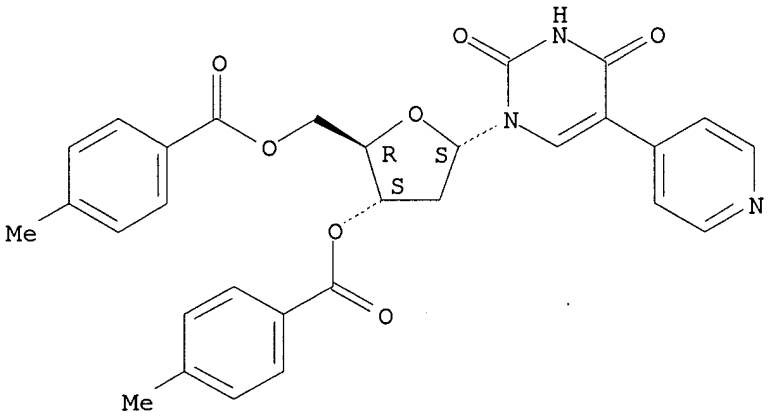
AB The title compds. [I; R1 = OH, NH2; R2 = (hetero)aryl, e.g. Q-Q2; X = O, S, Se, (un)substituted NH; R3 = H, OH, F, OMe; R4 = H, F, OH or its ether or ester residue, OMe, cyano, C.tplbond.CH, N3; R5 = OH or its ether or ester residue, (CH2)nP(O)(OM)2, (CH2)nP(O)(OM)CH2P(O)(OM)2; R6 = H, straight or branched C1-10 alkyl, halo, etc.; M = H, a pharmaceutically acceptable counterion; n = 0, 1], useful for treatment of infections by viruses requiring reverse transcriptase for replication, e.g. human immunodeficiency virus (HIV) and hepatitis B virus, were prepared Thus, silylation of 5-(2-thienyl)uracil (II) with hexamethyldisilazane in the presence of Me3SiCl and (NH4)2SO4 under reflux gave bis-trimethylsilylated II which was stirred overnight with 2-deoxy-3,5-di-O-p-toluoyl-D-ribofuranosyl chloride in ClCH2CH2Cl in the presence of mol. sieve 4A. The product was treated with MeONa in MeOH to give α- and β-I (R1 = R4 = R5 = OH, R2 = 2-thienyl, R3 = H). α-I in vitro showed IC50 of 0.05-10 μM against HIV in H9 cells. Analogously prepared and tested were addnl. 26 I. Cellular toxicity of I on H9 and F500 cells and inhibition of enzymes (e.g. HIV reverse transcriptase, hepatitis B virus DNA polymerase, and herpes simplex virus type 2 DNA polymerase) by I were also given.

IT **127235-51-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of pyrimidine nucleoside virucide)

RN 127235-51-2 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 1-[2-deoxy-3,5-bis-O-(4-methylbenzoyl)-α-D-erythro-pentofuranosyl]-5-(4-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

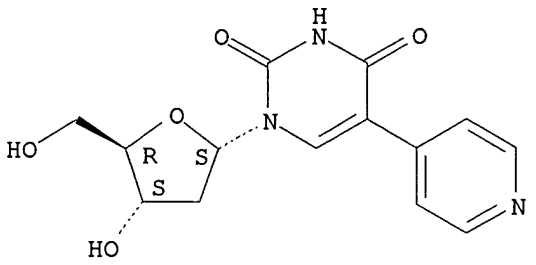


IT **127235-71-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as virucide)

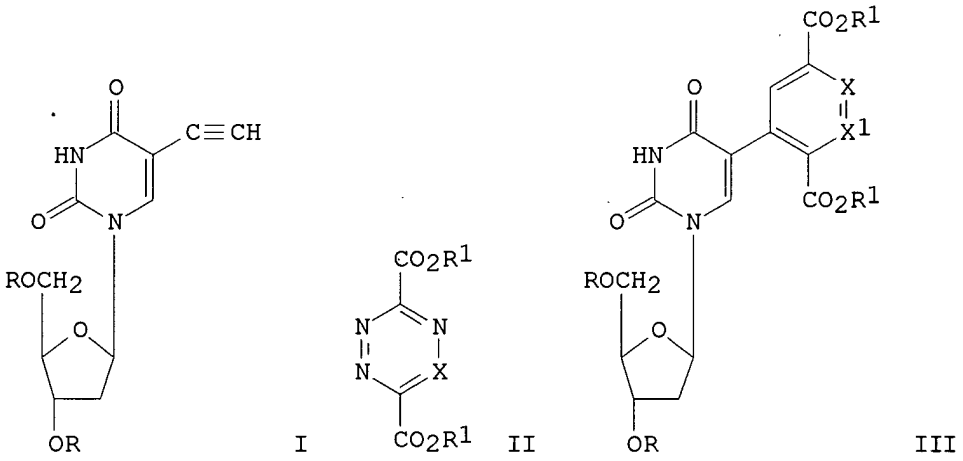
RN 127235-71-6 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 1-(2-deoxy-α-D-erythro-pentofuranosyl)-5-(4-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

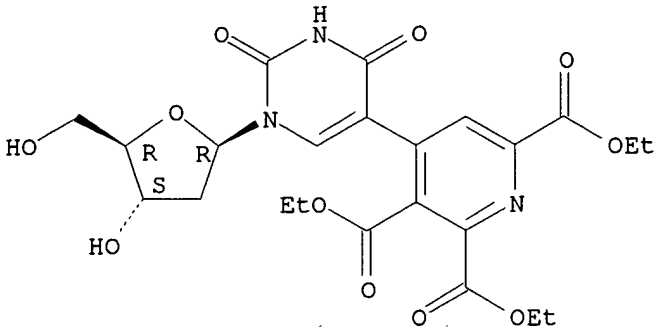


L3 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1986:130206 CAPLUS
DN 104:130206
TI Diels-Alder reactions of azadienes. A facile approach to the synthesis of pyridine- and pyridazine-substituted pyrimidine nucleosides
AU Maggiora, Linda; Mertes, Mathias P.
CS Dep. Med. Chem., Univ. Kansas, Lawrence, KS, 66045, USA
SO Journal of Organic Chemistry (1986), 51(6), 950-1
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 104:130206
GI



AB The Diels-Alder reaction of 5-ethynyl-2'-deoxyuridine I (R = H, Ac) with carboxylate II (R1 = Me; X = N) afforded 5-(3,6-dicarbomethoxypyridazin-4-yl)-2'-deoxyuridine III (R1 = Me, X = N) in 70% yield. Treatment of I with II (R1 = Et; X = X1 = CCO2Et) produced a 30% yield of III (R1 = Et; X = N, CCO2Et, X = CCO2Et, X1 = N).
IT **100021-03-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 100021-03-2 CAPLUS
CN 2,3,6-Pyridinetricarboxylic acid, 4-[1-(2-deoxy-β-D-erythro-pentofuranosyl)-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]-, triethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.


H
N
O
O
O
N
O
HO
R
R
S
HO
EtO
O
N
O
OEt
O
OEt

=>